



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:39 AM UTC

PDB ID : 1F51 / pdb_00001f51
Title : A TRANSIENT INTERACTION BETWEEN TWO PHOSPHORELAY PROTEINS TRAPPED IN A CRYSTAL LATTICE REVEALS THE MECHANISM OF MOLECULAR RECOGNITION AND PHOSPHOTRANSFER IN SINGAL TRANSDUCTION
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Deposited on : 2000-06-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

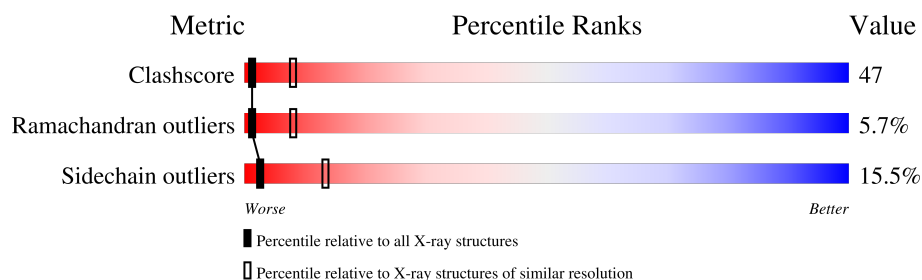
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	
1	B	182	
1	C	182	
1	D	182	
2	E	119	
2	F	119	
2	G	119	
2	H	119	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SPORULATION INITIATION PHOSPHOTRANSFERASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1489	949	250	283	7			
1	B	182	Total	C	N	O	S	6	0	0
			1504	959	253	285	7			
1	C	181	Total	C	N	O	S	0	0	0
			1481	945	249	280	7			
1	D	182	Total	C	N	O	S	6	0	0
			1497	955	252	283	7			

- Molecule 2 is a protein called SPORULATION INITIATION PHOSPHOTRANSFERASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	119	Total	C	N	O	S	0	0	0
			940	603	155	177	5			
2	F	119	Total	C	N	O	S	0	0	0
			950	609	156	180	5			
2	G	119	Total	C	N	O	S	0	0	0
			947	608	155	179	5			
2	H	119	Total	C	N	O	S	0	0	0
			940	603	155	177	5			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

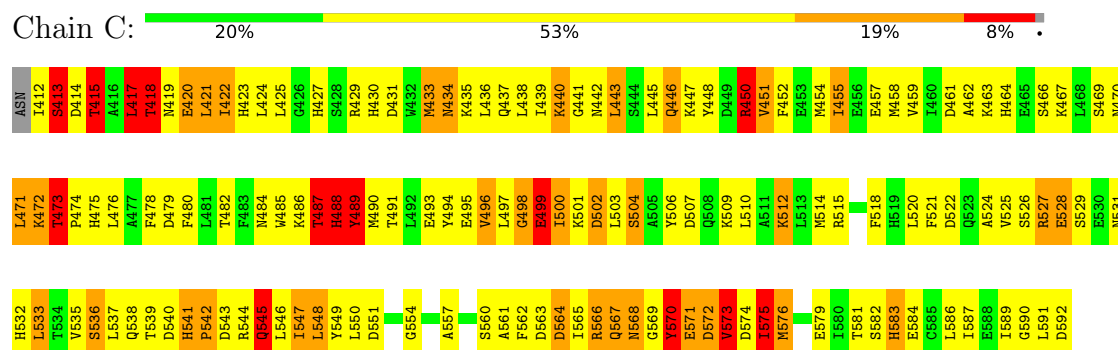
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



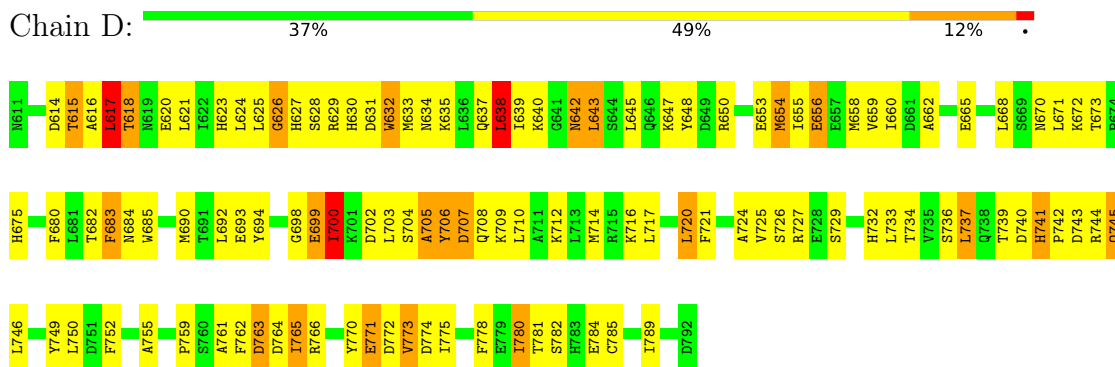
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



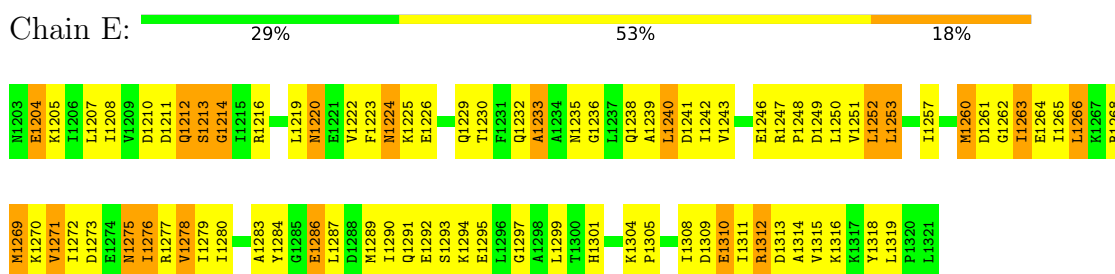
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



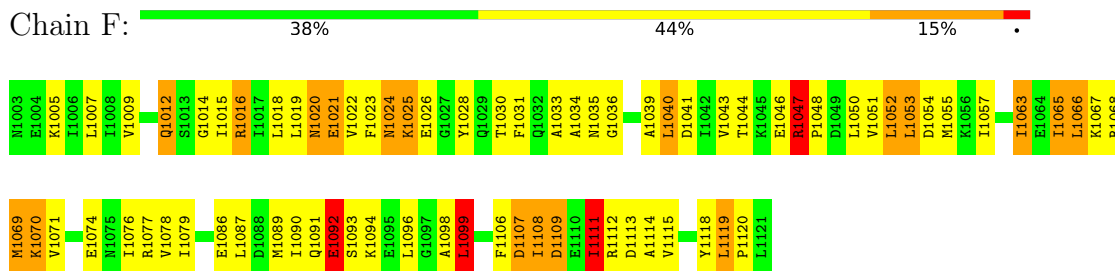
● Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



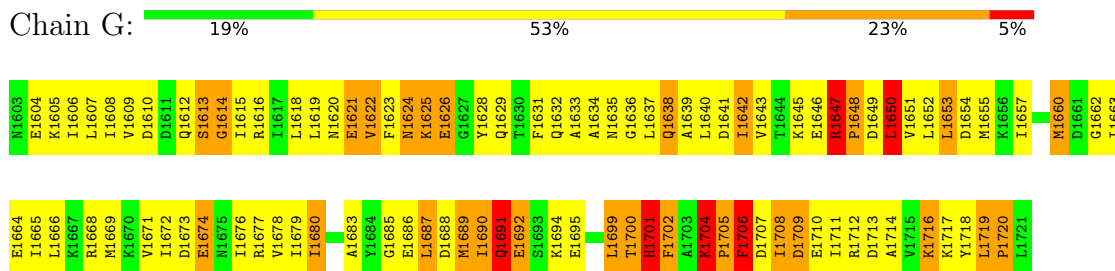
● Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



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El464	El465	El466	El467	El468	El469	El470	El471	El472	El473	El474	El475	El476	El477	El478	El479	El480	El481	El482	El483	El484	El485	El486	El487	El488	El489	El490	El491	El492	El493	El494	El495	El496	El497	El498	El499	El500	El501	El502	El503	El504	El505	El506	El507	El508	El509	El510	El511	El512	El513	El514	El515	El516	El517	El518	El519	El520	El521	El522	El523	El524	El525	El526	El527	El528	El529	El530	El531	El532	El533	El534	El535	El536	El537	El538	El539	El540	El541	El542	El543	El544	El545	El546	El547	El548	El549	El550	El551	El552	El553	El554	El555	El556	El557	El558	El559	El560	El561	El562	El563	El564	El565	El566	El567	El568	El569	El570	El571	El572	El573	El574	El575	El576	El577	El578	El579	El580	El581	El582	El583	El584	El585	El586	El587	El588	El589	El590	El591	El592	El593	El594	El595	El596	El597	El598	El599	El600	El601	El602	El603	El604	El605	El606	El607	El608	El609	El610	El611	El612	El613	El614	El615	El616	El617	El618	El619	El620	El621	El622	El623	El624	El625	El626	El627	El628	El629	El630	El631	El632	El633	El634	El635	El636	El637	El638	El639	El640	El641	El642	El643	El644	El645	El646	El647	El648	El649	El650	El651	El652	El653	El654	El655	El656	El657	El658	El659	El660	El661	El662	El663	El664	El665	El666	El667	El668	El669	El670	El671	El672	El673	El674	El675	El676	El677	El678	El679	El680	El681	El682	El683	El684	El685	El686	El687	El688	El689	El690	El691	El692	El693	El694	El695	El696	El697	El698	El699	El700	El701	El702	El703	El704	El705	El706	El707	El708	El709	El710	El711	El712	El713	El714	El715	El716	El717	El718	El719	El720	El721	El722	El723	El724	El725	El726	El727	El728	El729	El730	El731	El732	El733	El734	El735	El736	El737	El738	El739	El740	El741	El742	El743	El744	El745	El746	El747	El748	El749	El750	El751	El752	El753	El754	El755	El756	El757	El758	El759	El760	El761	El762	El763	El764	El765	El766	El767	El768	El769	El770	El771	El772	El773	El774	El775	El776	El777	El778	El779	El780	El781	El782	El783	El784	El785	El786	El787	El788	El789	El790	El791	El792	El793	El794	El795	El796	El797	El798	El799	El800	El801	El802	El803	El804	El805	El806	El807	El808	El809	El810	El811	El812	El813	El814	El815	El816	El817	El818	El819	El820	El821	El822	El823	El824	El825	El826	El827	El828	El829	El830	El831	El832	El833	El834	El835	El836	El837	El838	El839	El840	El841	El842	El843	El844	El845	El846	El847	El848	El849	El850	El851	El852	El853	El854	El855	El856	El857	El858	El859	El860	El861	El862	El863	El864	El865	El866	El867	El868	El869	El870	El871	El872	El873	El874	El875	El876	El877	El878	El879	El880	El881	El882	El883	El884	El885	El886	El887	El888	El889	El890	El891	El892	El893	El894	El895	El896	El897	El898	El899	El900	El901	El902	El903	El904	El905	El906	El907	El908	El909	El910	El911	El912	El913	El914	El915	El916	El917	El918	El919	El920	El921	El922	El923	El924	El925	El926	El927	El928	El929	El930	El931	El932	El933	El934	El935	El936	El937	El938	El939	El940	El941	El942	El943	El944	El945	El946	El947	El948	El949	El950	El951	El952	El953	El954	El955	El956	El957	El958	El959	El960	El961	El962	El963	El964	El965	El966	El967	El968	El969	El970	El971	El972	El973	El974	El975	El976	El977	El978	El979	El980	El981	El982	El983	El984	El985	El986	El987	El988	El989	El990	El991	El992	El993	El994	El995	El996	El997	El998	El999	El1000
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 117.77Å 170.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.7 (45.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	7.60	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.228 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/1522	1.12	14/2056 (0.7%)
1	B	0.59	1/1537 (0.1%)	1.16	13/2075 (0.6%)
1	C	0.56	0/1514	1.45	31/2045 (1.5%)
1	D	0.54	0/1530	1.14	14/2065 (0.7%)
2	E	0.54	0/951	1.11	6/1280 (0.5%)
2	F	0.60	0/961	1.22	10/1293 (0.8%)
2	G	0.63	1/958 (0.1%)	1.33	14/1289 (1.1%)
2	H	0.53	0/951	1.56	27/1280 (2.1%)
All	All	0.57	2/9924 (0.0%)	1.26	129/13383 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1704	LYS	C-O	-7.77	1.14	1.24
1	B	290	MET	SD-CE	-6.32	1.63	1.79

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	567	GLN	N-CA-C	-25.09	82.12	113.23
2	H	1469	MET	N-CA-C	-12.93	96.96	113.12
1	D	617	LEU	N-CA-C	-12.26	98.30	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1519	LEU	N-CA-C	-12.15	92.70	110.20
2	H	1466	LEU	N-CA-C	-11.57	97.30	112.68
1	A	13	SER	N-CA-C	11.03	122.35	108.45
2	G	1705	PRO	N-CA-C	-10.66	84.38	112.10
2	H	1476	ILE	N-CA-C	10.12	122.33	108.17
2	H	1516	LYS	N-CA-C	-10.09	97.74	111.96
1	D	699	GLU	N-CA-C	9.85	125.91	109.76
2	H	1517	LYS	N-CA-C	-9.84	95.44	110.10
1	C	488	HIS	N-CA-C	9.73	131.52	110.80
2	H	1494	LYS	N-CA-C	-9.07	101.36	111.07
1	C	473	THR	CA-C-N	8.83	128.42	119.24
1	C	473	THR	C-N-CA	8.83	128.42	119.24
2	H	1520	PRO	N-CA-C	8.62	130.22	112.47
1	C	570	TYR	N-CA-C	-8.59	97.78	109.54
1	C	414	ASP	N-CA-C	8.56	129.03	110.80
1	A	73	THR	CA-C-N	8.30	128.26	119.05
1	A	73	THR	C-N-CA	8.30	128.26	119.05
1	B	300	ILE	N-CA-C	8.24	126.48	109.34
1	A	168	ASN	N-CA-C	-8.19	93.36	110.80
2	F	1111	ILE	N-CA-C	-8.15	102.94	111.58
1	B	299	GLU	N-CA-C	8.15	122.24	110.10
1	C	473	THR	N-CA-C	-8.09	95.62	110.02
2	H	1515	VAL	N-CA-C	-8.05	105.17	112.90
2	G	1695	GLU	N-CA-C	-7.99	103.26	113.16
1	C	499	GLU	N-CA-C	7.78	127.37	110.80
2	G	1701	HIS	N-CA-C	-7.73	94.34	110.80
1	B	217	LEU	N-CA-C	-7.60	103.00	111.28
2	F	1078	VAL	N-CA-C	7.59	118.73	108.11
2	G	1605	LYS	N-CA-C	7.46	121.84	109.46
2	H	1430	THR	N-CA-C	7.44	120.60	110.55
1	A	14	ASP	N-CA-C	-7.35	95.14	110.80
1	B	361	ALA	N-CA-C	-7.26	104.42	113.28
1	C	471	LEU	N-CA-C	-7.22	102.26	113.02
1	B	365	ILE	N-CA-C	-7.09	101.68	111.89
1	C	413	SER	N-CA-C	7.08	125.88	110.80
1	C	497	LEU	N-CA-C	6.99	120.07	108.96
1	C	541	HIS	N-CA-C	6.94	119.47	109.48
1	C	569	GLY	N-CA-C	6.84	129.40	113.18
2	F	1092	GLU	N-CA-C	-6.78	96.37	110.80
1	D	709	LYS	N-CA-C	-6.73	103.87	111.14
2	G	1647	ARG	CA-C-N	6.66	128.05	120.85
2	G	1647	ARG	C-N-CA	6.66	128.05	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	643	LEU	N-CA-C	-6.65	103.85	112.23
2	H	1428	TYR	N-CA-C	6.64	124.94	110.80
2	H	1489	MET	N-CA-C	-6.62	105.33	113.41
1	C	545	GLN	N-CA-C	6.58	124.81	110.80
1	A	128	GLU	N-CA-C	-6.57	105.80	113.88
2	F	1047	ARG	CA-C-N	6.52	126.48	120.03
2	F	1047	ARG	C-N-CA	6.52	126.48	120.03
1	A	120	LEU	N-CA-C	-6.46	104.23	111.28
1	C	576	MET	N-CA-C	6.42	119.97	111.75
1	C	499	GLU	CA-C-N	6.41	129.09	120.50
1	C	499	GLU	C-N-CA	6.41	129.09	120.50
2	G	1678	VAL	N-CA-C	6.36	116.83	106.72
1	D	741	HIS	N-CA-C	6.34	117.79	109.93
2	H	1519	LEU	CA-C-N	6.30	127.71	119.84
2	H	1519	LEU	C-N-CA	6.30	127.71	119.84
1	C	488	HIS	CA-C-N	6.29	133.56	121.54
1	C	488	HIS	C-N-CA	6.29	133.56	121.54
2	F	1053	LEU	N-CA-C	6.24	119.03	107.99
1	A	141	HIS	CA-C-N	6.23	125.85	119.56
1	A	141	HIS	C-N-CA	6.23	125.85	119.56
1	A	61	ASP	N-CA-C	-6.21	104.43	111.14
1	B	250	ARG	N-CA-C	-6.17	104.56	111.28
1	A	176	MET	N-CA-C	6.10	118.89	111.82
2	H	1457	ILE	CA-C-N	6.07	125.98	119.85
2	H	1457	ILE	C-N-CA	6.07	125.98	119.85
2	G	1626	GLU	N-CA-C	-6.06	105.87	113.20
2	H	1490	ILE	N-CA-C	-6.06	103.56	112.04
1	C	450	ARG	N-CA-C	-6.05	104.80	111.82
1	B	216	ALA	N-CA-C	-5.97	105.91	113.43
2	F	1066	LEU	N-CA-C	-5.95	104.14	111.40
1	D	739	THR	N-CA-C	-5.94	106.37	113.97
2	H	1475	ASN	CA-C-N	-5.93	115.83	123.19
2	H	1475	ASN	C-N-CA	-5.93	115.83	123.19
1	D	665	GLU	N-CA-C	-5.93	104.90	111.36
1	C	527	ARG	N-CA-C	-5.87	104.74	112.72
1	C	422	ILE	N-CA-C	-5.85	106.78	111.81
1	C	512	LYS	N-CA-C	-5.84	104.60	110.97
1	C	417	LEU	N-CA-C	-5.82	102.65	111.56
2	F	1024	ASN	N-CA-C	-5.82	105.02	111.36
2	G	1648	PRO	N-CA-C	5.82	121.38	111.03
1	B	326	SER	N-CA-C	-5.77	102.76	110.55
2	F	1099	LEU	N-CA-C	5.77	117.57	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1497	GLY	N-CA-C	5.75	123.00	115.40
2	G	1685	GLY	N-CA-C	5.71	126.70	113.18
2	H	1461	ASP	N-CA-C	5.69	117.57	108.41
2	G	1610	ASP	N-CA-C	-5.68	101.33	110.14
2	H	1487	LEU	N-CA-C	5.66	122.86	110.80
1	C	563	ASP	N-CA-C	5.62	117.41	111.28
1	B	265	GLU	N-CA-C	-5.61	104.38	111.11
2	H	1473	ASP	N-CA-C	-5.58	97.78	107.49
2	E	1229	GLN	N-CA-C	-5.58	100.08	108.96
1	D	705	ALA	N-CA-C	5.54	118.03	111.33
1	D	645	LEU	N-CA-C	-5.53	106.38	113.02
2	G	1624	ASN	N-CA-C	-5.52	107.09	113.88
1	B	214	ASP	N-CA-C	-5.50	102.87	110.35
1	B	248	TYR	N-CA-C	5.50	122.51	110.80
2	E	1312	ARG	N-CA-C	-5.50	105.20	111.14
2	E	1271	VAL	N-CA-C	-5.49	105.61	113.07
2	H	1483	ALA	N-CA-C	-5.47	101.94	110.42
1	C	433	MET	N-CA-C	-5.46	105.23	111.07
1	C	420	GLU	N-CA-C	-5.43	105.27	111.14
1	D	706	TYR	N-CA-C	5.43	120.01	113.17
1	C	487	THR	N-CA-C	5.42	122.34	110.80
1	D	638	LEU	N-CA-C	-5.41	105.03	111.03
1	D	632	TRP	N-CA-C	-5.40	105.47	111.36
2	E	1283	ALA	N-CA-C	-5.38	100.92	109.96
1	A	126	SER	N-CA-C	-5.36	103.45	110.53
2	H	1427	GLY	N-CA-C	5.29	125.71	113.18
2	H	1453	LEU	N-CA-C	5.26	116.88	108.41
1	D	630	HIS	N-CA-C	5.26	116.70	110.97
2	F	1090	ILE	N-CA-C	-5.25	105.38	110.42
2	G	1642	ILE	N-CA-C	-5.20	105.47	110.72
2	G	1700	THR	N-CA-C	-5.20	99.73	110.80
1	C	489	TYR	N-CA-CB	5.19	119.26	110.49
1	A	65	GLU	N-CA-C	-5.18	104.89	111.11
2	H	1511	ILE	N-CA-C	-5.17	108.25	113.47
1	C	504	SER	N-CA-C	-5.14	105.67	111.28
2	E	1253	LEU	N-CA-C	5.13	116.88	108.52
1	B	276	LEU	N-CA-C	-5.12	105.59	111.07
1	B	257	GLU	N-CA-C	-5.10	104.99	111.11
2	E	1278	VAL	N-CA-C	5.08	115.22	108.11
1	A	163	ASP	N-CA-C	5.02	117.14	111.02
1	D	626	GLY	N-CA-C	-5.01	106.68	113.24
1	C	437	GLN	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	570	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1489	0	1437	87	0
1	B	1504	0	1463	120	0
1	C	1481	0	1419	179	0
1	D	1497	0	1449	123	1
2	E	940	0	970	89	1
2	F	950	0	987	84	0
2	G	947	0	983	170	0
2	H	940	0	970	112	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	9751	0	9678	914	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1465:ILE:O	2:H:1469:MET:HB2	1.40	1.19
1:C:520:LEU:HD13	1:C:565:ILE:HD11	1.27	1.15
1:C:544:ARG:HH21	1:C:592:ASP:HA	1.10	1.14
2:G:1677:ARG:HB3	2:G:1699:LEU:HD11	1.31	1.13
2:G:1683:ALA:HA	2:G:1704:LYS:HE3	1.28	1.13
1:C:500:ILE:HD12	1:C:500:ILE:H	1.11	1.10
2:G:1687:LEU:HA	2:G:1690:ILE:HB	1.26	1.10
1:D:699:GLU:HB2	1:D:700:ILE:HD12	1.35	1.08
1:C:433:MET:HE1	1:D:659:VAL:HA	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1609:VAL:HG21	2:G:1639:ALA:HB2	1.32	1.05
2:H:1477:ARG:HH12	2:H:1520:PRO:CA	1.70	1.04
1:C:544:ARG:NH2	1:C:592:ASP:HA	1.75	1.00
2:H:1477:ARG:HH12	2:H:1520:PRO:HA	1.26	0.98
2:F:1051:VAL:HG11	2:F:1069:MET:HE1	1.43	0.97
2:H:1449:ASP:O	2:H:1477:ARG:HG3	1.65	0.96
1:C:544:ARG:HH21	1:C:592:ASP:CA	1.78	0.96
1:C:500:ILE:H	1:C:500:ILE:CD1	1.73	0.95
1:C:514:MET:HE1	1:C:548:LEU:HD13	1.46	0.95
1:A:71:LEU:HB2	1:A:73:THR:HG22	1.48	0.94
2:G:1683:ALA:HA	2:G:1704:LYS:CE	1.97	0.94
2:E:1223:PHE:HE1	2:E:1315:VAL:HG21	1.32	0.94
2:E:1270:LYS:NZ	2:E:1297:GLY:HA3	1.83	0.93
2:G:1608:ILE:HG21	2:G:1619:LEU:HD12	1.51	0.92
2:F:1020:ASN:HB2	2:F:1030:THR:HG21	1.50	0.91
2:H:1468:ARG:HG3	2:H:1471:VAL:HG21	1.53	0.90
1:D:737:LEU:HD21	1:D:746:LEU:HD22	1.53	0.90
1:C:520:LEU:CD1	1:C:565:ILE:HD11	2.02	0.90
2:G:1699:LEU:H	2:G:1699:LEU:HD12	1.36	0.90
1:D:633:MET:HE3	2:H:1505:PRO:HD3	1.54	0.90
2:G:1690:ILE:C	2:G:1692:GLU:H	1.75	0.89
1:C:514:MET:HE1	1:C:548:LEU:CD1	2.02	0.89
2:E:1226:GLU:OE2	2:E:1312:ARG:HD2	1.72	0.89
2:E:1223:PHE:CE1	2:E:1315:VAL:HG21	2.06	0.89
1:C:546:LEU:HD12	1:C:591:LEU:HD12	1.53	0.88
2:E:1243:VAL:HA	2:E:1248:PRO:HD2	1.55	0.88
2:F:1020:ASN:C	2:F:1022:VAL:H	1.77	0.87
1:D:673:THR:HG22	1:D:707:ASP:HB2	1.58	0.86
2:H:1477:ARG:NH1	2:H:1520:PRO:HA	1.90	0.86
1:C:417:LEU:CD1	1:D:617:LEU:HB2	2.05	0.85
1:A:144:ARG:HH22	1:A:174:ASP:HB3	1.38	0.85
1:D:737:LEU:CD2	1:D:746:LEU:HD22	2.05	0.85
1:C:500:ILE:HD12	1:C:500:ILE:N	1.92	0.84
2:E:1286:GLU:O	2:E:1290:ILE:HG13	1.77	0.84
2:G:1680:ILE:HD13	2:G:1680:ILE:H	1.41	0.83
2:F:1055:MET:HB3	2:F:1089:MET:CE	2.08	0.83
2:H:1468:ARG:HA	2:H:1471:VAL:HG23	1.59	0.83
1:B:381:THR:HG23	1:B:384:GLU:H	1.43	0.83
2:H:1407:LEU:HD13	2:H:1442:ILE:HG21	1.58	0.83
2:G:1683:ALA:CA	2:G:1704:LYS:HE3	2.08	0.83
1:B:337:LEU:HD22	1:B:348:LEU:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1713:ASP:HA	2:G:1716:LYS:HG3	1.61	0.83
2:G:1677:ARG:HD2	2:G:1699:LEU:HD21	1.60	0.83
2:G:1606:ILE:HD13	2:G:1650:LEU:HD13	1.61	0.82
1:B:344:ARG:CZ	1:B:376:MET:HE3	2.08	0.82
1:B:356:PHE:HB2	1:B:359:PRO:HG3	1.60	0.82
1:C:520:LEU:HD13	1:C:565:ILE:CD1	2.09	0.82
1:C:421:LEU:O	1:C:425:LEU:HG	1.80	0.82
1:B:344:ARG:HH12	1:B:374:ASP:CG	1.86	0.82
1:D:668:LEU:HD12	1:D:671:LEU:HD12	1.61	0.81
2:G:1707:ASP:O	2:G:1710:GLU:HG2	1.79	0.81
2:G:1607:LEU:HD12	2:G:1608:ILE:H	1.45	0.81
1:A:71:LEU:HB2	1:A:73:THR:CG2	2.11	0.80
1:C:482:THR:HB	1:C:486:LYS:HE3	1.61	0.80
1:C:538:GLN:OE1	1:C:547:ILE:HD11	1.81	0.80
1:C:541:HIS:HD2	1:C:544:ARG:H	1.30	0.80
2:F:1051:VAL:HG11	2:F:1069:MET:CE	2.11	0.80
1:C:415:THR:HG23	1:D:675:HIS:NE2	1.98	0.79
2:E:1226:GLU:OE1	2:E:1316:LYS:HD3	1.82	0.79
1:A:141:HIS:CD2	1:A:143:ASP:H	2.01	0.79
1:C:574:ASP:O	1:C:576:MET:HG3	1.82	0.79
2:F:1055:MET:HB3	2:F:1089:MET:HE2	1.63	0.79
1:D:708:GLN:HB3	1:D:712:LYS:HE2	1.64	0.78
2:E:1207:LEU:HD13	2:E:1242:ILE:HG21	1.65	0.78
2:G:1609:VAL:HG22	2:G:1633:ALA:HB3	1.63	0.78
1:A:144:ARG:NH2	1:A:174:ASP:HB3	1.98	0.78
2:E:1275:ASN:HD22	2:E:1275:ASN:H	1.28	0.78
2:H:1490:ILE:O	2:H:1494:LYS:HB2	1.83	0.77
2:G:1612:GLN:HB3	2:G:1615:ILE:HD12	1.67	0.77
1:A:141:HIS:HD2	1:A:144:ARG:H	1.32	0.76
2:G:1607:LEU:O	2:G:1608:ILE:HD13	1.86	0.76
2:G:1613:SER:O	2:G:1615:ILE:N	2.19	0.76
1:D:703:LEU:HD23	1:D:706:TYR:CD1	2.21	0.75
2:E:1270:LYS:HZ2	2:E:1297:GLY:HA3	1.49	0.75
2:H:1426:GLU:OE2	2:H:1512:ARG:HD2	1.86	0.75
2:H:1517:LYS:O	2:H:1518:TYR:HB2	1.85	0.75
1:B:338:GLN:NE2	1:B:347:ILE:HD12	2.01	0.75
2:H:1477:ARG:HH22	2:H:1520:PRO:HA	1.52	0.75
1:B:356:PHE:CB	1:B:359:PRO:HG3	2.16	0.74
1:D:717:LEU:HA	1:D:720:LEU:HD11	1.66	0.74
2:F:1054:ASP:HB3	2:F:1057:ILE:HD11	1.68	0.74
2:H:1436:GLY:HA3	2:H:1460:MET:SD	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:LEU:HD12	1:C:548:LEU:HB3	1.70	0.74
1:D:741:HIS:ND1	1:D:742:PRO:HD2	2.01	0.74
2:H:1490:ILE:HD12	2:H:1490:ILE:H	1.52	0.74
1:C:433:MET:CE	1:D:659:VAL:HA	2.16	0.74
2:G:1633:ALA:HA	2:G:1638:GLN:HE21	1.53	0.74
2:G:1690:ILE:HG22	2:G:1691:GLN:N	2.02	0.74
1:D:616:ALA:C	1:D:618:THR:H	1.94	0.74
2:G:1717:LYS:HE2	2:G:1718:TYR:CZ	2.22	0.74
1:D:637:GLN:NE2	2:H:1506:PHE:H	1.87	0.73
1:D:639:ILE:O	1:D:643:LEU:HB2	1.88	0.73
2:G:1700:THR:HG23	2:G:1701:HIS:H	1.52	0.73
2:H:1466:LEU:HD11	2:H:1498:ALA:HB2	1.68	0.73
2:G:1700:THR:HG23	2:G:1701:HIS:N	2.04	0.73
1:C:498:GLY:O	1:C:539:THR:OG1	2.05	0.73
2:G:1608:ILE:HA	2:G:1652:LEU:O	1.88	0.73
1:B:344:ARG:NH1	1:B:374:ASP:OD1	2.20	0.73
2:F:1020:ASN:C	2:F:1022:VAL:N	2.47	0.73
2:G:1633:ALA:HA	2:G:1638:GLN:NE2	2.03	0.73
1:C:570:TYR:HD2	1:C:573:VAL:HG11	1.51	0.72
1:D:690:MET:HE1	1:D:733:LEU:CD2	2.19	0.72
2:H:1452:LEU:HB3	2:H:1481:MET:CE	2.18	0.72
1:C:471:LEU:HB2	1:C:473:THR:HG22	1.70	0.72
1:D:617:LEU:O	1:D:617:LEU:HG	1.87	0.72
1:C:445:LEU:O	1:C:446:GLN:HB2	1.90	0.72
1:D:770:TYR:HB3	1:D:773:VAL:CG2	2.19	0.72
1:B:337:LEU:HD22	1:B:348:LEU:CD1	2.20	0.71
2:E:1250:LEU:HD12	2:E:1277:ARG:O	1.90	0.71
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.55	0.71
2:F:1092:GLU:O	2:F:1096:LEU:HD12	1.91	0.71
2:G:1660:MET:HE3	2:G:1665:ILE:HD13	1.71	0.71
2:H:1470:LYS:NZ	2:H:1496:LEU:HD22	2.05	0.71
1:C:537:LEU:HG	1:C:546:LEU:HD21	1.72	0.71
2:E:1250:LEU:HD21	2:E:1279:ILE:HD12	1.72	0.71
1:D:780:ILE:HG12	1:D:780:ILE:O	1.91	0.71
2:E:1294:LYS:HE2	2:E:1299:LEU:O	1.91	0.71
2:H:1465:ILE:O	2:H:1469:MET:CB	2.31	0.71
2:F:1055:MET:HE3	2:F:1089:MET:HE2	1.73	0.70
2:H:1519:LEU:HG	2:H:1520:PRO:HD2	1.73	0.70
2:H:1413:SER:O	2:H:1417:ILE:HG13	1.92	0.70
1:B:308:GLN:O	1:B:312:LYS:HB2	1.91	0.70
1:D:703:LEU:HD22	1:D:746:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:C	1:B:248:TYR:H	2.00	0.70
1:B:268:LEU:HA	1:B:271:LEU:HD12	1.72	0.70
2:H:1512:ARG:O	2:H:1515:VAL:HG22	1.92	0.70
2:F:1020:ASN:HB2	2:F:1030:THR:CG2	2.21	0.70
2:G:1607:LEU:HD11	2:G:1633:ALA:HB3	1.73	0.70
2:G:1687:LEU:C	2:G:1689:MET:H	1.99	0.70
2:H:1466:LEU:HD23	2:H:1469:MET:HE2	1.72	0.70
1:D:637:GLN:NE2	2:H:1506:PHE:N	2.40	0.69
2:E:1208:ILE:HD13	2:E:1252:LEU:HD12	1.74	0.69
1:C:567:GLN:O	1:C:568:ASN:HB2	1.91	0.69
2:F:1051:VAL:HG21	2:F:1069:MET:HE2	1.74	0.69
2:E:1268:ARG:O	2:E:1272:ILE:HG13	1.93	0.69
2:H:1477:ARG:NH2	2:H:1520:PRO:HA	2.08	0.69
1:B:381:THR:HG21	1:B:384:GLU:HG3	1.73	0.69
1:D:716:LYS:HD2	1:D:770:TYR:CE1	2.28	0.69
1:D:637:GLN:HE21	2:H:1506:PHE:N	1.91	0.69
1:D:703:LEU:O	1:D:704:SER:C	2.35	0.69
2:G:1713:ASP:OD1	2:G:1716:LYS:HE2	1.93	0.69
2:H:1477:ARG:HH12	2:H:1520:PRO:CB	2.06	0.69
1:D:699:GLU:HB2	1:D:700:ILE:CD1	2.17	0.69
2:H:1452:LEU:HB3	2:H:1481:MET:HE2	1.72	0.69
1:A:170:TYR:O	1:A:173:VAL:HG22	1.93	0.68
2:G:1636:GLY:O	2:G:1640:LEU:HD13	1.94	0.68
1:B:281:LEU:HD23	1:B:294:TYR:OH	1.94	0.68
1:C:506:TYR:CZ	1:C:545:GLN:NE2	2.62	0.68
1:C:521:PHE:O	1:C:525:VAL:HG22	1.92	0.68
2:E:1223:PHE:C	2:E:1225:LYS:H	1.99	0.68
2:E:1311:ILE:O	2:E:1315:VAL:HG13	1.93	0.68
1:C:464:HIS:ND1	1:C:496:VAL:HG23	2.09	0.68
1:D:673:THR:HG22	1:D:707:ASP:CB	2.24	0.68
2:F:1053:LEU:CD1	2:F:1065:ILE:HD11	2.24	0.68
1:C:522:ASP:O	1:C:527:ARG:NH2	2.25	0.68
1:B:267:LYS:HE2	1:B:299:GLU:HG2	1.75	0.68
1:C:417:LEU:HD13	1:D:617:LEU:HB2	1.74	0.68
1:D:638:LEU:O	1:D:642:ASN:OD1	2.12	0.68
2:G:1643:VAL:HG21	2:G:1669:MET:HE3	1.76	0.68
2:G:1654:ASP:O	2:G:1657:ILE:HG13	1.95	0.67
1:C:541:HIS:CD2	1:C:544:ARG:H	2.11	0.67
2:E:1265:ILE:O	2:E:1269:MET:HB2	1.94	0.67
2:E:1275:ASN:H	2:E:1275:ASN:ND2	1.92	0.67
1:C:442:ASN:HA	1:C:445:LEU:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1264:GLU:O	2:E:1268:ARG:HG3	1.94	0.67
1:C:412:ILE:O	1:C:413:SER:HB2	1.93	0.67
2:G:1690:ILE:C	2:G:1692:GLU:N	2.42	0.67
2:G:1677:ARG:CB	2:G:1699:LEU:HD11	2.18	0.67
1:D:633:MET:CE	2:H:1505:PRO:HD3	2.24	0.67
2:F:1099:LEU:HG	2:F:1118:TYR:CD1	2.30	0.67
1:D:655:ILE:O	1:D:659:VAL:HG23	1.95	0.66
2:E:1270:LYS:HZ1	2:E:1297:GLY:HA3	1.58	0.66
1:A:63:LYS:O	1:A:67:LYS:HG3	1.95	0.66
1:C:417:LEU:HD12	1:D:617:LEU:HD12	1.76	0.66
1:C:544:ARG:CZ	1:C:592:ASP:HA	2.26	0.66
1:D:654:MET:O	1:D:658:MET:HG3	1.95	0.66
1:C:464:HIS:CE1	1:C:496:VAL:H	2.13	0.66
1:A:29:ARG:HD3	1:B:265:GLU:OE1	1.96	0.66
1:A:144:ARG:HH22	1:A:174:ASP:CB	2.08	0.66
1:A:141:HIS:HD2	1:A:143:ASP:H	1.44	0.66
1:D:629:ARG:O	1:D:633:MET:HG2	1.96	0.66
2:G:1614:GLY:O	2:G:1618:LEU:N	2.24	0.66
1:B:255:ILE:O	1:B:259:VAL:HG23	1.95	0.66
2:G:1680:ILE:HD13	2:G:1680:ILE:N	2.11	0.66
2:G:1701:HIS:O	2:G:1702:PHE:HD2	1.78	0.66
2:E:1253:LEU:CD2	2:E:1265:ILE:HD11	2.26	0.65
1:D:781:THR:HG23	1:D:784:GLU:H	1.61	0.65
2:E:1257:ILE:HD12	2:E:1260:MET:CE	2.27	0.65
1:A:65:GLU:HG3	1:A:81:LEU:HD21	1.78	0.65
2:H:1477:ARG:NH1	2:H:1520:PRO:CA	2.51	0.65
1:C:570:TYR:HD2	1:C:573:VAL:CG1	2.09	0.65
1:C:490:MET:CE	1:C:533:LEU:HD12	2.25	0.65
2:H:1461:ASP:OD1	2:H:1464:GLU:OE1	2.14	0.65
1:B:288:HIS:HD2	1:B:322:ASP:OD2	1.79	0.65
2:G:1609:VAL:O	2:G:1657:ILE:HD11	1.97	0.65
2:G:1618:LEU:O	2:G:1618:LEU:HD23	1.96	0.65
1:D:620:GLU:O	1:D:623:HIS:HB3	1.97	0.65
1:B:220:GLU:O	1:B:224:LEU:HG	1.96	0.65
1:B:375:ILE:HG22	1:B:375:ILE:O	1.96	0.65
1:D:716:LYS:HZ2	1:D:770:TYR:HD1	1.46	0.64
2:G:1636:GLY:HA2	2:G:1665:ILE:HG12	1.79	0.64
2:G:1677:ARG:NH2	2:G:1720:PRO:HG2	2.12	0.64
1:A:48:TYR:O	1:A:52:PHE:HD1	1.79	0.64
1:A:34:ASN:O	1:A:37:GLN:HB3	1.96	0.64
2:E:1220:ASN:O	2:E:1224:ASN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1077:ARG:NE	2:F:1120:PRO:HG2	2.13	0.64
2:H:1420:ASN:ND2	2:H:1432:GLN:HE21	1.94	0.64
2:H:1436:GLY:O	2:H:1440:LEU:HD22	1.97	0.64
1:A:154:GLY:O	1:A:183:HIS:HB3	1.97	0.64
2:E:1251:VAL:HB	2:E:1278:VAL:HG22	1.80	0.64
2:H:1477:ARG:CZ	2:H:1520:PRO:HA	2.27	0.64
1:C:436:LEU:HD23	1:C:439:ILE:HD12	1.79	0.64
1:C:445:LEU:HD21	2:G:1618:LEU:HD21	1.80	0.64
1:D:775:ILE:HG13	1:D:775:ILE:O	1.97	0.64
2:H:1420:ASN:ND2	2:H:1432:GLN:NE2	2.46	0.64
1:C:472:LYS:C	1:C:474:PRO:HD3	2.22	0.64
2:H:1511:ILE:O	2:H:1511:ILE:HG13	1.98	0.64
1:B:306:TYR:CD2	1:B:391:LEU:HD22	2.33	0.64
1:C:531:ASN:OD1	1:C:554:GLY:HA3	1.98	0.64
1:C:570:TYR:O	1:C:570:TYR:CD2	2.51	0.64
2:E:1236:GLY:O	2:E:1240:LEU:HD22	1.98	0.63
1:B:344:ARG:NH2	1:B:376:MET:HE3	2.12	0.63
1:C:445:LEU:HD11	2:G:1618:LEU:HG	1.81	0.63
1:C:509:LYS:NZ	1:C:592:ASP:OD2	2.32	0.63
1:A:141:HIS:CD2	1:A:144:ARG:H	2.15	0.63
2:E:1250:LEU:HD11	2:E:1279:ILE:HG13	1.80	0.63
2:H:1467:LYS:O	2:H:1470:LYS:HB2	1.99	0.63
2:E:1310:GLU:HA	2:E:1313:ASP:HB2	1.81	0.63
1:A:167:GLN:O	1:A:168:ASN:CG	2.41	0.63
1:B:338:GLN:HE21	1:B:341:HIS:HB2	1.63	0.63
2:H:1490:ILE:HD12	2:H:1490:ILE:N	2.13	0.63
2:H:1490:ILE:HG21	2:H:1501:HIS:CD2	2.34	0.63
1:A:44:SER:CB	2:E:1308:ILE:HG21	2.29	0.62
1:C:490:MET:HE3	1:C:533:LEU:HD12	1.81	0.62
1:C:510:LEU:CD2	1:C:591:LEU:HD11	2.29	0.62
2:E:1287:LEU:HA	2:E:1290:ILE:HD12	1.81	0.62
2:G:1633:ALA:HB1	2:G:1638:GLN:HB3	1.80	0.62
1:B:214:ASP:OD2	1:B:214:ASP:N	2.28	0.62
1:C:435:LYS:HB3	1:C:458:MET:HE2	1.80	0.62
1:C:443:LEU:HD22	1:C:451:VAL:HG21	1.81	0.62
2:F:1055:MET:HB3	2:F:1089:MET:HE1	1.81	0.62
2:H:1463:ILE:HG22	2:H:1464:GLU:N	2.15	0.62
1:B:366:ARG:NH2	1:C:579:GLU:OE1	2.32	0.62
1:B:370:TYR:O	1:B:371:GLU:O	2.18	0.62
1:D:690:MET:HE1	1:D:733:LEU:HD22	1.80	0.62
1:C:570:TYR:CD2	1:C:573:VAL:HG11	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:GLN:NE2	2:H:1505:PRO:HA	2.15	0.62
2:G:1608:ILE:CG2	2:G:1619:LEU:HD12	2.28	0.62
2:H:1465:ILE:O	2:H:1465:ILE:HD12	2.00	0.61
1:C:575:ILE:HG12	1:C:575:ILE:O	2.00	0.61
2:G:1666:LEU:C	2:G:1666:LEU:HD23	2.25	0.61
2:G:1614:GLY:O	2:G:1618:LEU:HB2	2.01	0.61
1:C:488:HIS:ND1	1:C:488:HIS:N	2.47	0.61
2:G:1621:GLU:HG3	2:G:1622:VAL:N	2.15	0.61
2:G:1672:ILE:HG22	2:G:1673:ASP:OD1	2.00	0.61
2:G:1650:LEU:HD23	2:G:1651:VAL:N	2.15	0.61
2:F:1021:GLU:HG2	2:F:1025:LYS:NZ	2.16	0.61
2:G:1609:VAL:HA	2:G:1633:ALA:O	2.01	0.61
1:A:43:LEU:HD12	1:B:252:PHE:CZ	2.36	0.61
2:E:1207:LEU:HB3	2:E:1251:VAL:HG22	1.81	0.61
2:H:1449:ASP:O	2:H:1477:ARG:CG	2.44	0.60
2:H:1468:ARG:HG3	2:H:1471:VAL:CG2	2.29	0.60
1:B:250:ARG:O	1:B:253:GLU:HB2	2.02	0.60
1:B:367:GLN:HG2	1:B:367:GLN:O	2.00	0.60
1:B:310:LEU:HD22	1:B:348:LEU:HD22	1.83	0.60
2:G:1687:LEU:HD13	2:G:1687:LEU:H	1.66	0.60
2:G:1653:LEU:HD12	2:G:1657:ILE:HD11	1.84	0.60
2:E:1261:ASP:HB3	2:E:1264:GLU:HB2	1.83	0.60
2:G:1613:SER:O	2:G:1616:ARG:N	2.35	0.60
1:A:39:ILE:O	1:A:43:LEU:HB2	2.01	0.60
1:B:266:SER:O	1:B:270:ASN:ND2	2.34	0.60
1:C:487:THR:C	1:C:488:HIS:ND1	2.60	0.60
1:C:510:LEU:HD21	1:C:591:LEU:CD1	2.32	0.60
2:G:1666:LEU:O	2:G:1669:MET:HB2	2.01	0.60
2:G:1691:GLN:HG3	2:G:1694:LYS:HD3	1.84	0.60
1:B:352:PHE:C	1:B:352:PHE:CD2	2.79	0.60
2:E:1250:LEU:HD12	2:E:1251:VAL:H	1.67	0.60
1:B:306:TYR:HD2	1:B:391:LEU:HD22	1.66	0.59
1:B:300:ILE:HD11	2:E:1287:LEU:HD12	1.84	0.59
1:C:573:VAL:O	1:C:573:VAL:CG2	2.49	0.59
2:E:1250:LEU:HA	2:E:1277:ARG:O	2.03	0.59
2:G:1686:GLU:O	2:G:1690:ILE:HG13	2.02	0.59
1:C:544:ARG:HG2	1:C:592:ASP:O	2.02	0.59
2:G:1628:TYR:CE1	2:G:1719:LEU:HG	2.36	0.59
2:E:1265:ILE:C	2:E:1265:ILE:HD12	2.27	0.59
2:G:1609:VAL:HG12	2:G:1657:ILE:CD1	2.33	0.59
1:D:698:GLY:HA3	1:D:740:ASP:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:TYR:OH	1:B:345:GLN:NE2	2.35	0.59
2:G:1609:VAL:HG12	2:G:1657:ILE:HD11	1.85	0.59
2:G:1633:ALA:HB1	2:G:1638:GLN:CB	2.32	0.59
1:B:381:THR:CG2	1:B:384:GLU:H	2.16	0.59
1:D:770:TYR:O	1:D:771:GLU:HB2	2.01	0.58
2:G:1677:ARG:HB3	2:G:1699:LEU:CD1	2.21	0.58
1:C:431:ASP:O	1:C:434:ASN:HB2	2.03	0.58
1:D:631:ASP:HA	1:D:634:ASN:HB2	1.85	0.58
1:C:441:GLY:O	1:C:445:LEU:HG	2.03	0.58
1:C:526:SER:C	1:C:528:GLU:H	2.11	0.58
2:H:1507:ASP:O	2:H:1509:ASP:N	2.36	0.58
1:C:573:VAL:HB	1:C:589:ILE:CG2	2.33	0.58
2:G:1620:ASN:CG	2:G:1632:GLN:HE21	2.12	0.58
1:D:670:ASN:O	1:D:700:ILE:CG2	2.52	0.58
2:E:1249:ASP:HB3	2:E:1319:LEU:HD11	1.86	0.58
2:F:1070:LYS:HG2	2:F:1076:ILE:CG2	2.33	0.58
2:G:1620:ASN:O	2:G:1624:ASN:HB2	2.04	0.58
1:C:554:GLY:O	1:C:583:HIS:HB3	2.03	0.58
1:C:574:ASP:O	1:C:576:MET:N	2.37	0.58
1:D:690:MET:HE1	1:D:733:LEU:HD23	1.85	0.58
2:F:1053:LEU:HD13	2:F:1065:ILE:HD11	1.85	0.58
2:F:1050:LEU:HD12	2:F:1077:ARG:CB	2.34	0.58
2:G:1607:LEU:HD11	2:G:1633:ALA:CB	2.34	0.58
2:H:1468:ARG:HA	2:H:1471:VAL:CG2	2.31	0.58
1:D:759:PRO:HB2	1:D:780:ILE:HD11	1.86	0.57
1:D:762:PHE:O	1:D:765:ILE:HG22	2.03	0.57
1:A:129:SER:OG	1:A:155:ALA:HB3	2.04	0.57
1:D:640:LYS:O	1:D:643:LEU:HB3	2.05	0.57
2:H:1441:ASP:O	2:H:1445:LYS:HG2	2.05	0.57
2:F:1055:MET:HE3	2:F:1089:MET:CE	2.35	0.57
2:G:1713:ASP:HA	2:G:1716:LYS:CG	2.33	0.57
2:H:1468:ARG:CG	2:H:1471:VAL:HG21	2.31	0.57
1:A:137:LEU:HD11	1:A:146:LEU:HD21	1.87	0.57
1:B:263:LYS:HG2	2:E:1284:TYR:CE2	2.39	0.57
2:F:1036:GLY:O	2:F:1040:LEU:HD22	2.04	0.57
2:G:1613:SER:O	2:G:1614:GLY:C	2.48	0.57
2:H:1517:LYS:O	2:H:1518:TYR:CB	2.53	0.57
1:D:744:ARG:NH2	1:D:774:ASP:OD2	2.38	0.57
2:F:1091:GLN:NE2	2:F:1094:LYS:HD3	2.20	0.57
2:G:1711:ILE:O	2:G:1714:ALA:HB3	2.05	0.57
1:D:729:SER:OG	1:D:755:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LEU:HD12	1:D:617:LEU:HB2	1.86	0.57
1:A:164:ASP:O	1:A:168:ASN:HB2	2.05	0.56
1:B:238:LEU:O	1:B:242:ASN:HB2	2.04	0.56
1:A:103:LEU:HD13	1:A:146:LEU:HD11	1.86	0.56
1:B:363:ASP:OD1	1:B:363:ASP:O	2.23	0.56
1:C:495:GLU:HB3	1:C:536:SER:HB3	1.88	0.56
1:D:716:LYS:NZ	1:D:770:TYR:HD1	2.02	0.56
2:H:1470:LYS:HZ3	2:H:1496:LEU:HD22	1.70	0.56
1:B:238:LEU:HD21	2:F:1014:GLY:HA3	1.88	0.56
2:F:1047:ARG:HG2	2:F:1047:ARG:HH11	1.70	0.56
1:B:349:TYR:C	1:B:350:LEU:HD12	2.30	0.56
1:C:573:VAL:HA	1:C:590:GLY:O	2.05	0.56
2:E:1257:ILE:HB	2:E:1260:MET:HE2	1.88	0.56
2:F:1020:ASN:O	2:F:1022:VAL:N	2.38	0.56
2:H:1408:ILE:HD12	2:H:1452:LEU:HD22	1.86	0.56
1:C:451:VAL:HG11	1:D:643:LEU:HD21	1.87	0.56
2:G:1655:MET:HE1	2:G:1663:ILE:HD13	1.87	0.56
2:H:1433:ALA:HB1	2:H:1438:GLN:HB2	1.88	0.56
1:C:412:ILE:O	1:C:413:SER:CB	2.54	0.56
1:C:459:VAL:O	1:C:462:ALA:HB3	2.05	0.56
1:C:522:ASP:OD1	1:C:527:ARG:NH2	2.39	0.56
1:D:775:ILE:HG22	1:D:789:ILE:HG12	1.87	0.56
2:E:1313:ASP:O	2:E:1316:LYS:HB2	2.06	0.56
2:G:1634:ALA:H	2:G:1638:GLN:NE2	2.03	0.56
2:F:1091:GLN:HE22	2:F:1094:LYS:HD3	1.70	0.56
2:G:1650:LEU:C	2:G:1650:LEU:CD2	2.79	0.56
1:B:263:LYS:HG2	2:E:1284:TYR:CZ	2.41	0.55
1:B:362:PHE:CD1	1:B:378:PHE:HZ	2.23	0.55
1:C:564:ASP:OD1	1:C:567:GLN:OE1	2.25	0.55
2:E:1289:MET:O	2:E:1293:SER:HB3	2.06	0.55
2:F:1053:LEU:HD11	2:F:1065:ILE:HD11	1.88	0.55
2:G:1623:PHE:HE1	2:G:1712:ARG:HA	1.68	0.55
2:G:1626:GLU:OE1	2:G:1626:GLU:HA	2.05	0.55
2:G:1707:ASP:HB3	2:G:1710:GLU:CD	2.31	0.55
2:H:1512:ARG:C	2:H:1514:ALA:H	2.14	0.55
2:F:1026:GLU:HG3	2:F:1112:ARG:HD2	1.88	0.55
2:G:1690:ILE:O	2:G:1692:GLU:N	2.40	0.55
1:B:346:LEU:HD11	1:B:348:LEU:HD13	1.89	0.55
2:E:1204:GLU:HA	2:E:1204:GLU:OE1	2.06	0.55
2:E:1257:ILE:HD12	2:E:1260:MET:HE1	1.89	0.55
2:H:1431:PHE:HB3	2:H:1442:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:670:ASN:O	1:D:700:ILE:HG22	2.06	0.55
2:F:1053:LEU:HD11	2:F:1065:ILE:CD1	2.37	0.55
1:B:235:LYS:HB3	1:B:258:MET:CE	2.37	0.55
1:C:490:MET:HA	1:C:531:ASN:O	2.05	0.55
1:C:586:LEU:HD23	1:C:587:ILE:N	2.22	0.55
1:A:138:GLN:OE1	1:A:147:ILE:HD11	2.08	0.54
1:D:703:LEU:HD21	1:D:746:LEU:HG	1.88	0.54
2:F:1021:GLU:O	2:F:1025:LYS:HD3	2.07	0.54
1:A:116:LYS:O	1:A:120:LEU:HG	2.06	0.54
1:C:544:ARG:NE	1:C:592:ASP:HA	2.23	0.54
2:E:1243:VAL:HA	2:E:1248:PRO:CD	2.33	0.54
2:H:1408:ILE:HG21	2:H:1419:LEU:HD12	1.88	0.54
2:H:1453:LEU:HG	2:H:1455:MET:SD	2.47	0.54
1:B:276:LEU:O	1:B:279:ASP:HB2	2.07	0.54
1:C:442:ASN:OD1	1:C:454:MET:HE1	2.07	0.54
1:B:328:GLU:O	1:B:328:GLU:HG3	2.04	0.54
2:H:1404:GLU:HB2	2:H:1428:TYR:HD1	1.72	0.54
1:C:544:ARG:HE	1:C:592:ASP:HA	1.73	0.54
1:D:770:TYR:HB3	1:D:773:VAL:HG21	1.89	0.54
1:A:37:GLN:OE1	2:E:1305:PRO:HA	2.08	0.54
1:A:50:ARG:O	1:A:54:MET:HG3	2.08	0.54
1:D:716:LYS:NZ	1:D:770:TYR:CD1	2.72	0.54
1:B:238:LEU:CD2	2:F:1014:GLY:HA3	2.38	0.54
1:C:506:TYR:CE2	1:C:545:GLN:NE2	2.76	0.54
2:F:1115:VAL:O	2:F:1119:LEU:HB2	2.08	0.54
2:E:1226:GLU:OE2	2:E:1312:ARG:CD	2.49	0.54
2:H:1443:VAL:HA	2:H:1448:PRO:HD2	1.90	0.54
1:B:239:ILE:O	1:B:243:LEU:HB2	2.08	0.54
1:B:374:ASP:OD1	1:B:374:ASP:O	2.26	0.54
1:C:445:LEU:HD13	1:C:447:LYS:HE2	1.90	0.54
2:G:1700:THR:O	2:G:1701:HIS:HB3	2.08	0.54
2:G:1663:ILE:O	2:G:1666:LEU:HB3	2.08	0.53
1:B:344:ARG:NH1	1:B:374:ASP:CG	2.63	0.53
1:C:541:HIS:NE2	1:C:543:ASP:HB2	2.22	0.53
2:G:1692:GLU:C	2:G:1694:LYS:H	2.15	0.53
1:A:126:SER:HB3	1:A:155:ALA:HB3	1.89	0.53
1:C:502:ASP:O	1:C:503:LEU:HD23	2.08	0.53
2:F:1077:ARG:HG2	2:F:1077:ARG:HH11	1.73	0.53
2:G:1607:LEU:HA	2:G:1631:PHE:O	2.09	0.53
2:G:1608:ILE:HD12	2:G:1619:LEU:HD13	1.90	0.53
2:H:1512:ARG:C	2:H:1514:ALA:N	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1016:ARG:HH12	2:F:1034:ALA:HB2	1.74	0.53
2:F:1019:LEU:O	2:F:1022:VAL:HB	2.09	0.53
2:F:1050:LEU:HD12	2:F:1077:ARG:HB2	1.90	0.53
1:A:123:GLN:O	1:A:123:GLN:HG3	2.09	0.53
2:H:1490:ILE:CG2	2:H:1501:HIS:CD2	2.92	0.53
1:C:451:VAL:O	1:C:452:PHE:C	2.51	0.53
1:C:571:GLU:N	1:C:571:GLU:OE2	2.41	0.53
1:B:268:LEU:HD12	1:B:271:LEU:HD12	1.90	0.53
1:C:544:ARG:HH21	1:C:592:ASP:N	2.07	0.53
1:D:624:LEU:O	1:D:627:HIS:N	2.40	0.53
2:G:1692:GLU:C	2:G:1694:LYS:N	2.63	0.53
2:E:1253:LEU:HD22	2:E:1265:ILE:HD11	1.91	0.53
2:F:1054:ASP:HB3	2:F:1057:ILE:CD1	2.37	0.53
2:F:1070:LYS:HD2	2:F:1096:LEU:O	2.09	0.53
2:F:1111:ILE:O	2:F:1114:ALA:HB3	2.09	0.53
2:E:1211:ASP:HB3	2:E:1257:ILE:HG12	1.91	0.53
2:E:1311:ILE:O	2:E:1315:VAL:HG22	2.09	0.53
2:G:1643:VAL:O	2:G:1647:ARG:HA	2.08	0.53
1:B:337:LEU:N	1:B:337:LEU:HD23	2.24	0.52
2:E:1223:PHE:C	2:E:1225:LYS:N	2.60	0.52
1:A:72:LYS:C	1:A:74:PRO:HD3	2.35	0.52
1:B:343:ASP:O	1:B:344:ARG:HB2	2.10	0.52
1:C:494:TYR:HA	1:C:535:VAL:O	2.08	0.52
1:D:708:GLN:O	1:D:712:LYS:HG3	2.09	0.52
2:F:1028:TYR:CE1	2:F:1119:LEU:HD21	2.45	0.52
2:H:1459:GLY:O	2:H:1460:MET:C	2.52	0.52
1:C:488:HIS:O	1:C:489:TYR:CG	2.62	0.52
2:G:1700:THR:CG2	2:G:1701:HIS:H	2.15	0.52
1:B:308:GLN:NE2	1:B:308:GLN:HA	2.24	0.52
1:B:336:SER:HB2	1:B:349:TYR:HB2	1.91	0.52
2:G:1607:LEU:HD21	2:G:1639:ALA:HA	1.91	0.52
1:C:476:LEU:HD22	1:C:510:LEU:CD1	2.39	0.52
2:G:1655:MET:HE1	2:G:1663:ILE:CD1	2.40	0.52
2:H:1423:PHE:CE1	2:H:1515:VAL:HG11	2.45	0.52
1:A:154:GLY:N	1:A:183:HIS:O	2.42	0.52
1:D:724:ALA:HB2	1:D:761:ALA:HB3	1.92	0.52
2:F:1036:GLY:O	2:F:1039:ALA:HB3	2.10	0.52
2:G:1676:ILE:O	2:G:1676:ILE:HG23	2.10	0.52
1:C:488:HIS:C	1:C:489:TYR:CD1	2.88	0.52
2:G:1708:ILE:O	2:G:1710:GLU:N	2.43	0.52
1:C:450:ARG:NH1	1:C:457:GLU:OE1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:ARG:NE	1:D:654:MET:HE3	2.24	0.52
2:G:1620:ASN:ND2	2:G:1632:GLN:HE21	2.08	0.52
2:G:1687:LEU:CD1	2:G:1687:LEU:N	2.73	0.52
2:H:1490:ILE:H	2:H:1490:ILE:CD1	2.21	0.52
1:A:44:SER:C	1:A:46:GLN:H	2.16	0.51
1:B:343:ASP:O	1:B:344:ARG:CB	2.57	0.51
1:C:572:ASP:CG	1:C:573:VAL:H	2.18	0.51
1:D:637:GLN:HE22	2:H:1506:PHE:H	1.55	0.51
1:A:144:ARG:NH1	1:A:176:MET:HE3	2.24	0.51
1:A:162:PHE:O	1:A:166:ARG:HG3	2.10	0.51
1:B:306:TYR:CE2	1:B:391:LEU:HB3	2.45	0.51
2:F:1028:TYR:HE1	2:F:1119:LEU:HD21	1.75	0.51
2:G:1655:MET:HB3	2:G:1689:MET:HE2	1.93	0.51
1:D:781:THR:CG2	1:D:784:GLU:HB2	2.40	0.51
2:G:1609:VAL:O	2:G:1609:VAL:HG12	2.10	0.51
2:G:1691:GLN:CG	2:G:1694:LYS:HD3	2.40	0.51
2:G:1718:TYR:O	2:G:1720:PRO:HD3	2.11	0.51
2:H:1405:LYS:HD3	2:H:1446:GLU:OE1	2.11	0.51
1:C:490:MET:HE1	1:C:533:LEU:HD12	1.93	0.51
1:D:700:ILE:HD12	1:D:700:ILE:N	2.26	0.51
2:E:1273:ASP:O	2:E:1276:ILE:HB	2.11	0.51
2:F:1012:GLN:HB3	2:F:1015:ILE:HD12	1.93	0.51
2:F:1052:LEU:HD12	2:F:1079:ILE:HB	1.93	0.51
2:H:1410:ASP:O	2:H:1416:ARG:HD3	2.11	0.51
2:H:1512:ARG:O	2:H:1514:ALA:N	2.38	0.51
1:B:353:HIS:HA	1:B:384:GLU:HA	1.92	0.51
1:C:424:LEU:HD13	1:D:621:LEU:HD22	1.93	0.51
1:D:627:HIS:O	1:D:628:SER:C	2.54	0.51
2:E:1314:ALA:O	2:E:1318:TYR:HD2	1.94	0.51
2:E:1247:ARG:NH2	2:E:1272:ILE:O	2.43	0.51
1:D:616:ALA:C	1:D:618:THR:N	2.63	0.51
2:F:1067:LYS:HG2	2:F:1096:LEU:HD22	1.93	0.51
2:G:1633:ALA:HB2	2:G:1642:ILE:HD12	1.93	0.51
2:G:1713:ASP:O	2:G:1716:LYS:HB2	2.11	0.51
1:B:381:THR:OG1	1:B:382:SER:N	2.42	0.50
1:D:703:LEU:CD2	1:D:746:LEU:HD11	2.42	0.50
2:H:1416:ARG:HD2	2:H:1433:ALA:O	2.11	0.50
2:H:1423:PHE:O	2:H:1428:TYR:HB2	2.11	0.50
1:C:514:MET:O	1:C:518:PHE:N	2.38	0.50
1:A:22:ILE:HD11	1:B:274:PRO:O	2.11	0.50
2:G:1638:GLN:O	2:G:1642:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ILE:HD12	1:B:212:ILE:N	2.26	0.50
1:B:344:ARG:NH1	1:B:390:GLY:HA3	2.26	0.50
2:G:1607:LEU:HD12	2:G:1631:PHE:O	2.12	0.50
1:A:19:ASN:OD1	1:B:274:PRO:HB3	2.11	0.50
2:H:1459:GLY:O	2:H:1460:MET:O	2.30	0.50
1:B:290:MET:CE	1:B:321:PHE:CB	2.90	0.50
1:C:541:HIS:HD2	1:C:544:ARG:N	2.03	0.50
2:H:1449:ASP:C	2:H:1477:ARG:HG3	2.32	0.50
1:C:538:GLN:HB3	1:C:547:ILE:HG13	1.94	0.50
2:H:1454:ASP:HA	2:H:1481:MET:HB2	1.94	0.50
1:C:524:ALA:HB2	1:C:561:ALA:HB3	1.94	0.49
2:E:1222:VAL:HG21	2:E:1308:ILE:HD11	1.94	0.49
2:F:1005:LYS:HD3	2:F:1046:GLU:O	2.11	0.49
1:A:167:GLN:O	1:A:168:ASN:CB	2.60	0.49
1:C:476:LEU:HD22	1:C:510:LEU:HD12	1.93	0.49
1:D:703:LEU:O	1:D:706:TYR:N	2.39	0.49
2:G:1647:ARG:HG2	2:G:1673:ASP:OD2	2.12	0.49
2:H:1450:LEU:HD12	2:H:1477:ARG:O	2.11	0.49
1:C:502:ASP:OD1	1:C:502:ASP:C	2.55	0.49
2:E:1314:ALA:O	2:E:1318:TYR:CD2	2.65	0.49
2:H:1404:GLU:HB2	2:H:1428:TYR:CD1	2.47	0.49
2:H:1509:ASP:CG	2:H:1512:ARG:HH22	2.20	0.49
1:B:310:LEU:O	1:B:314:MET:HG2	2.12	0.49
1:B:375:ILE:O	1:B:375:ILE:CG2	2.61	0.49
1:C:418:THR:HA	1:C:421:LEU:HD12	1.95	0.49
1:C:450:ARG:HD2	1:C:454:MET:HG3	1.94	0.49
1:C:482:THR:HA	1:C:485:TRP:CE3	2.47	0.49
1:D:647:LYS:NZ	2:H:1421:GLU:OE1	2.45	0.49
2:F:1020:ASN:ND2	2:F:1024:ASN:HD21	2.09	0.49
2:F:1077:ARG:NE	2:F:1120:PRO:CG	2.75	0.49
2:G:1606:ILE:HD13	2:G:1650:LEU:CD1	2.40	0.49
2:G:1687:LEU:C	2:G:1689:MET:N	2.66	0.49
2:H:1452:LEU:HD21	2:H:1511:ILE:HD11	1.94	0.49
1:C:489:TYR:CD1	1:C:522:ASP:OD1	2.66	0.49
1:D:626:GLY:HA2	1:D:629:ARG:NH2	2.28	0.49
2:H:1408:ILE:CD1	2:H:1452:LEU:HD22	2.43	0.49
1:A:59:VAL:O	1:A:63:LYS:HB2	2.12	0.49
1:C:443:LEU:CD2	1:C:451:VAL:HG21	2.43	0.49
1:C:564:ASP:O	1:C:567:GLN:HB3	2.12	0.49
1:C:482:THR:HG22	1:C:485:TRP:CE3	2.47	0.49
1:C:526:SER:HA	1:C:557:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD21	1:B:391:LEU:CD1	2.42	0.49
1:B:360:SER:O	1:B:363:ASP:OD1	2.31	0.49
1:C:445:LEU:O	1:C:446:GLN:CB	2.61	0.49
2:E:1208:ILE:HD13	2:E:1252:LEU:CD1	2.42	0.49
1:C:442:ASN:ND2	1:C:447:LYS:HD2	2.28	0.49
1:C:448:TYR:CE2	1:D:648:TYR:CE1	3.00	0.49
1:D:682:THR:O	1:D:683:PHE:C	2.55	0.49
2:F:1020:ASN:ND2	2:F:1024:ASN:ND2	2.61	0.49
2:F:1021:GLU:HG2	2:F:1025:LYS:HZ1	1.76	0.49
2:F:1031:PHE:CE1	2:F:1046:GLU:HG3	2.47	0.49
2:H:1455:MET:HG2	2:H:1480:ILE:HB	1.93	0.49
1:B:325:VAL:HA	1:B:356:PHE:HA	1.94	0.48
1:C:510:LEU:HD21	1:C:591:LEU:HD11	1.92	0.48
2:G:1634:ALA:H	2:G:1638:GLN:CD	2.21	0.48
2:H:1407:LEU:HB3	2:H:1451:VAL:HG22	1.94	0.48
1:B:344:ARG:HH11	1:B:390:GLY:HA3	1.77	0.48
1:D:614:ASP:O	1:D:615:THR:OG1	2.20	0.48
2:F:1093:SER:O	2:F:1098:ALA:CB	2.61	0.48
2:G:1701:HIS:O	2:G:1702:PHE:CD2	2.62	0.48
1:A:72:LYS:HB3	1:A:104:SER:HB3	1.96	0.48
1:B:239:ILE:HG22	1:B:240:LYS:N	2.27	0.48
1:B:264:HIS:HA	1:B:267:LYS:HB2	1.95	0.48
1:B:313:LEU:O	1:B:316:LYS:HB3	2.13	0.48
2:H:1420:ASN:HD22	2:H:1432:GLN:NE2	2.10	0.48
1:C:427:HIS:HB3	1:C:485:TRP:CD1	2.49	0.48
1:C:455:ILE:O	1:C:459:VAL:HG23	2.13	0.48
1:C:475:HIS:O	1:C:479:ASP:OD1	2.32	0.48
2:E:1223:PHE:HE1	2:E:1315:VAL:CG2	2.16	0.48
2:G:1637:LEU:HB3	2:G:1641:ASP:OD2	2.14	0.48
1:B:246:GLN:C	1:B:248:TYR:N	2.69	0.48
1:B:333:LEU:HD12	1:B:334:THR:N	2.29	0.48
1:A:14:ASP:HB3	1:A:17:LEU:HB3	1.95	0.48
1:B:212:ILE:HD12	1:B:212:ILE:H	1.79	0.48
2:E:1240:LEU:O	2:E:1241:ASP:C	2.57	0.48
2:F:1016:ARG:HH12	2:F:1034:ALA:CB	2.26	0.48
2:G:1717:LYS:HE2	2:G:1718:TYR:CE2	2.48	0.48
1:B:375:ILE:HG13	1:B:389:ILE:HG12	1.96	0.48
1:D:717:LEU:HA	1:D:720:LEU:CD1	2.40	0.48
2:E:1291:GLN:O	2:E:1292:GLU:C	2.57	0.48
2:G:1612:GLN:CB	2:G:1615:ILE:HD12	2.42	0.48
2:G:1635:ASN:H	2:G:1638:GLN:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:PHE:HB3	1:D:694:TYR:CE2	2.49	0.47
2:E:1213:SER:O	2:E:1214:GLY:C	2.57	0.47
2:G:1691:GLN:C	2:G:1694:LYS:HB3	2.39	0.47
2:G:1708:ILE:C	2:G:1710:GLU:H	2.21	0.47
1:D:752:PHE:HB3	1:D:785:CYS:HB3	1.96	0.47
2:E:1275:ASN:ND2	2:E:1275:ASN:N	2.62	0.47
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.27	0.47
2:G:1606:ILE:HG12	2:G:1650:LEU:HB3	1.95	0.47
2:G:1628:TYR:CZ	2:G:1719:LEU:HG	2.49	0.47
1:A:171:GLU:HB3	1:A:172:ASP:H	1.47	0.47
1:D:693:GLU:O	1:D:734:THR:HA	2.14	0.47
1:D:706:TYR:OH	1:D:745:GLN:HG2	2.14	0.47
1:D:762:PHE:CD1	1:D:778:PHE:HZ	2.33	0.47
2:G:1615:ILE:O	2:G:1619:LEU:N	2.43	0.47
1:B:344:ARG:NH1	1:B:374:ASP:OD2	2.47	0.47
1:C:572:ASP:C	1:C:573:VAL:HG13	2.40	0.47
1:D:638:LEU:HB3	1:D:654:MET:SD	2.55	0.47
2:F:1041:ASP:O	2:F:1044:THR:N	2.44	0.47
2:G:1647:ARG:CZ	2:G:1673:ASP:OD1	2.62	0.47
1:B:218:THR:HG22	1:B:219:ASN:N	2.28	0.47
1:B:364:ASP:OD1	1:B:364:ASP:C	2.58	0.47
1:B:378:PHE:C	1:B:378:PHE:CD2	2.93	0.47
1:C:549:TYR:C	1:C:550:LEU:HD12	2.39	0.47
2:E:1312:ARG:NH1	2:E:1312:ARG:HB3	2.29	0.47
2:G:1638:GLN:O	2:G:1642:ILE:CG1	2.62	0.47
2:H:1407:LEU:O	2:H:1451:VAL:HA	2.15	0.47
1:D:627:HIS:HB3	1:D:685:TRP:CE2	2.50	0.47
2:G:1679:ILE:HG23	2:G:1701:HIS:HA	1.96	0.47
1:C:480:PHE:CE2	1:C:514:MET:HG2	2.50	0.47
2:E:1291:GLN:O	2:E:1295:GLU:HB2	2.15	0.47
1:A:119:HIS:O	1:A:123:GLN:HG2	2.15	0.47
1:B:229:ARG:O	1:B:233:MET:HG2	2.15	0.47
1:D:635:LYS:O	1:D:639:ILE:HG13	2.15	0.47
1:D:710:LEU:O	1:D:714:MET:HG2	2.15	0.47
2:F:1046:GLU:O	2:F:1047:ARG:C	2.57	0.47
1:A:77:ALA:O	1:A:81:LEU:HD12	2.15	0.46
1:A:121:PHE:C	1:A:123:GLN:H	2.23	0.46
2:G:1717:LYS:HG3	2:G:1718:TYR:N	2.29	0.46
2:H:1416:ARG:HG2	2:H:1432:GLN:HB3	1.97	0.46
1:C:506:TYR:HE1	1:C:592:ASP:HB2	1.80	0.46
1:D:749:TYR:C	1:D:750:LEU:HD12	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1224:ASN:HD22	2:E:1224:ASN:HA	1.50	0.46
1:A:101:LYS:HE2	1:A:103:LEU:HD21	1.98	0.46
1:D:693:GLU:HB2	1:D:732:HIS:CE1	2.51	0.46
2:F:1009:VAL:HG22	2:F:1033:ALA:HB3	1.97	0.46
2:G:1691:GLN:CD	2:G:1694:LYS:HD3	2.40	0.46
2:H:1473:ASP:OD2	2:H:1476:ILE:HG13	2.15	0.46
1:A:24:LEU:HD13	1:B:221:LEU:HD22	1.97	0.46
1:A:67:LYS:HB3	1:A:100:ILE:HD11	1.95	0.46
1:A:121:PHE:O	1:A:125:VAL:HG13	2.15	0.46
1:A:133:LEU:HD22	1:A:134:THR:N	2.31	0.46
1:A:158:ASP:OD1	1:A:160:SER:OG	2.32	0.46
1:C:417:LEU:HG	1:C:421:LEU:HD11	1.98	0.46
1:C:502:ASP:O	1:C:502:ASP:OD1	2.33	0.46
1:D:650:ARG:HE	1:D:654:MET:HE3	1.80	0.46
2:F:1107:ASP:C	2:F:1109:ASP:H	2.23	0.46
2:G:1645:LYS:HE3	2:G:1646:GLU:HG2	1.97	0.46
2:G:1708:ILE:C	2:G:1710:GLU:N	2.72	0.46
1:B:378:PHE:HD2	1:B:378:PHE:O	1.99	0.46
1:C:445:LEU:HD11	2:G:1618:LEU:CG	2.44	0.46
2:G:1690:ILE:HG22	2:G:1691:GLN:H	1.78	0.46
2:H:1490:ILE:O	2:H:1494:LYS:CB	2.59	0.46
2:G:1613:SER:C	2:G:1615:ILE:N	2.73	0.46
1:C:451:VAL:CG1	1:D:643:LEU:HD21	2.45	0.46
1:B:335:VAL:HA	1:B:349:TYR:O	2.14	0.46
1:B:240:LYS:HZ3	2:F:1106:PHE:C	2.24	0.46
1:A:40:LYS:HA	1:A:43:LEU:HB2	1.98	0.46
1:B:290:MET:CE	1:B:321:PHE:HB2	2.45	0.46
1:D:647:LYS:NZ	2:H:1421:GLU:OE2	2.49	0.46
2:F:1063:ILE:O	2:F:1067:LYS:HG3	2.15	0.46
1:C:471:LEU:HB2	1:C:473:THR:CG2	2.41	0.45
1:D:763:ASP:O	1:D:764:ASP:C	2.59	0.45
2:F:1093:SER:HA	2:F:1096:LEU:HD12	1.98	0.45
2:H:1509:ASP:HB3	2:H:1512:ARG:NH2	2.30	0.45
1:A:73:THR:HG23	1:A:73:THR:O	2.17	0.45
1:B:341:HIS:CD2	1:B:347:ILE:HD11	2.51	0.45
1:B:381:THR:HG1	1:B:382:SER:H	1.65	0.45
1:C:420:GLU:C	1:C:422:ILE:N	2.73	0.45
1:C:544:ARG:HE	1:C:592:ASP:CA	2.29	0.45
2:E:1262:GLY:O	2:E:1266:LEU:HB2	2.16	0.45
1:C:549:TYR:N	1:C:549:TYR:CD2	2.83	0.45
1:D:692:LEU:HD12	1:D:693:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1220:ASN:OD1	2:E:1232:GLN:NE2	2.35	0.45
2:F:1024:ASN:HB3	2:G:1625:LYS:HG3	1.98	0.45
2:G:1700:THR:CG2	2:G:1701:HIS:N	2.70	0.45
1:D:703:LEU:O	1:D:705:ALA:N	2.50	0.45
1:D:653:GLU:O	1:D:655:ILE:N	2.50	0.45
2:G:1677:ARG:HH22	2:G:1720:PRO:HG2	1.81	0.45
1:D:653:GLU:C	1:D:655:ILE:N	2.74	0.45
1:C:440:LYS:CE	2:G:1705:PRO:HB2	2.47	0.45
1:D:682:THR:OG1	1:D:683:PHE:N	2.49	0.45
1:D:765:ILE:CG2	1:D:766:ARG:N	2.79	0.45
2:G:1618:LEU:O	2:G:1622:VAL:HG23	2.17	0.45
2:G:1639:ALA:O	2:G:1643:VAL:HG23	2.17	0.45
2:G:1643:VAL:HA	2:G:1648:PRO:CD	2.46	0.45
2:G:1666:LEU:C	2:G:1666:LEU:CD2	2.90	0.45
2:H:1443:VAL:HA	2:H:1448:PRO:CD	2.47	0.45
1:A:93:GLU:CG	1:A:132:HIS:NE2	2.79	0.45
1:A:141:HIS:HB2	1:A:147:ILE:HD13	1.97	0.45
1:C:486:LYS:O	1:C:487:THR:OG1	2.33	0.45
1:C:570:TYR:HB3	1:C:573:VAL:CG2	2.47	0.45
1:D:781:THR:OG1	1:D:782:SER:N	2.42	0.45
2:E:1293:SER:OG	2:E:1294:LYS:N	2.50	0.45
2:G:1692:GLU:C	2:G:1692:GLU:OE2	2.60	0.45
2:H:1425:LYS:HB2	2:H:1426:GLU:OE1	2.16	0.45
1:C:495:GLU:O	1:C:536:SER:HA	2.17	0.45
2:F:1018:LEU:O	2:F:1022:VAL:HG23	2.16	0.45
2:G:1604:GLU:HB2	2:G:1628:TYR:HD1	1.82	0.45
2:G:1650:LEU:HD23	2:G:1650:LEU:C	2.42	0.45
2:H:1471:VAL:O	2:H:1471:VAL:HG12	2.17	0.45
1:C:544:ARG:CG	1:C:592:ASP:O	2.64	0.44
1:C:566:ARG:HA	1:C:566:ARG:HD3	1.66	0.44
2:H:1445:LYS:O	2:H:1446:GLU:HG2	2.17	0.44
1:A:93:GLU:O	1:A:134:THR:HA	2.17	0.44
1:B:290:MET:HE1	1:B:321:PHE:CB	2.47	0.44
1:B:338:GLN:NE2	1:B:341:HIS:HB2	2.32	0.44
2:G:1638:GLN:HE21	2:G:1638:GLN:HB3	1.59	0.44
1:C:567:GLN:CG	1:C:568:ASN:N	2.79	0.44
2:F:1026:GLU:CG	2:F:1112:ARG:HD2	2.47	0.44
2:G:1637:LEU:O	2:G:1638:GLN:C	2.58	0.44
2:G:1677:ARG:NH2	2:G:1720:PRO:CG	2.79	0.44
1:A:59:VAL:O	1:A:59:VAL:HG12	2.17	0.44
1:B:314:MET:O	1:B:315:ARG:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1618:LEU:HD23	2:G:1618:LEU:C	2.43	0.44
2:G:1687:LEU:H	2:G:1687:LEU:CD1	2.30	0.44
1:A:89:TYR:CD1	1:A:127:ARG:NH2	2.86	0.44
1:C:420:GLU:C	1:C:422:ILE:H	2.26	0.44
1:C:528:GLU:O	1:C:529:SER:HB2	2.17	0.44
1:A:42:ASN:H	1:A:42:ASN:HD22	1.65	0.44
1:B:352:PHE:CE2	1:B:356:PHE:CZ	3.06	0.44
1:C:547:ILE:HD12	1:C:549:TYR:OH	2.18	0.44
1:C:570:TYR:HB3	1:C:573:VAL:HG21	1.99	0.44
1:A:38:LEU:HD21	2:E:1214:GLY:HA3	2.00	0.44
1:A:38:LEU:O	1:A:42:ASN:ND2	2.51	0.44
1:B:221:LEU:HG	1:B:225:LEU:HD12	1.99	0.44
1:B:307:ASP:O	1:B:309:LYS:N	2.50	0.44
1:C:550:LEU:HB2	1:C:587:ILE:HB	1.99	0.44
1:D:628:SER:O	1:D:632:TRP:HB2	2.18	0.44
2:G:1662:GLY:HA2	2:G:1665:ILE:HG22	1.99	0.44
2:H:1443:VAL:O	2:H:1447:ARG:HA	2.18	0.44
1:A:124:ALA:O	1:A:157:ALA:N	2.47	0.44
1:A:137:LEU:CD1	1:A:146:LEU:HD21	2.47	0.44
1:D:680:PHE:HZ	1:D:714:MET:HE2	1.83	0.44
1:D:703:LEU:C	1:D:705:ALA:N	2.73	0.44
2:F:1052:LEU:HD12	2:F:1052:LEU:HA	1.76	0.44
1:C:445:LEU:HB2	1:C:447:LYS:HG3	2.00	0.44
1:C:470:ASN:O	1:C:500:ILE:HG22	2.18	0.44
1:A:54:MET:O	1:A:55:ILE:C	2.61	0.43
1:A:64:HIS:O	1:A:65:GLU:C	2.61	0.43
1:B:350:LEU:HB2	1:B:387:ILE:HB	2.00	0.43
1:B:383:HIS:HB2	1:C:584:GLU:OE1	2.17	0.43
1:C:573:VAL:O	1:C:573:VAL:HG23	2.15	0.43
1:C:575:ILE:O	1:C:575:ILE:CG1	2.65	0.43
1:D:706:TYR:CD1	1:D:706:TYR:N	2.86	0.43
2:H:1514:ALA:HA	2:H:1517:LYS:HB3	2.00	0.43
2:H:1516:LYS:O	2:H:1519:LEU:N	2.51	0.43
1:A:40:LYS:HD3	2:E:1305:PRO:HB2	2.00	0.43
1:C:464:HIS:ND1	1:C:496:VAL:N	2.54	0.43
2:G:1655:MET:HG2	2:G:1680:ILE:HB	2.00	0.43
2:G:1677:ARG:HD2	2:G:1699:LEU:CD2	2.40	0.43
1:A:73:THR:N	1:A:74:PRO:HD3	2.32	0.43
1:B:370:TYR:O	1:B:371:GLU:C	2.61	0.43
1:D:771:GLU:O	1:D:772:ASP:HB2	2.17	0.43
2:G:1641:ASP:O	2:G:1645:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HD2	1:A:102:ASP:OD2	2.19	0.43
1:C:499:GLU:O	1:C:539:THR:OG1	2.32	0.43
2:F:1005:LYS:HB2	2:F:1048:PRO:HA	2.01	0.43
2:F:1091:GLN:O	2:F:1092:GLU:HB2	2.17	0.43
2:H:1440:LEU:HD12	2:H:1472:ILE:HD13	1.99	0.43
2:H:1441:ASP:O	2:H:1442:ILE:C	2.60	0.43
1:A:178:PHE:HA	1:A:186:LEU:O	2.18	0.43
1:B:290:MET:HE1	1:B:321:PHE:HB2	2.01	0.43
1:B:333:LEU:HD13	1:B:352:PHE:HB2	1.99	0.43
2:E:1232:GLN:O	2:E:1233:ALA:HB2	2.18	0.43
2:F:1093:SER:O	2:F:1098:ALA:HB2	2.18	0.43
1:A:125:VAL:O	1:A:127:ARG:NH1	2.52	0.43
1:C:442:ASN:HA	1:C:445:LEU:CD1	2.47	0.43
1:C:566:ARG:C	1:C:568:ASN:N	2.50	0.43
2:G:1609:VAL:HG22	2:G:1633:ALA:CB	2.42	0.43
2:F:1020:ASN:CB	2:F:1030:THR:HG21	2.35	0.43
2:G:1674:GLU:H	2:G:1674:GLU:HG2	1.41	0.43
2:H:1437:LEU:O	2:H:1438:GLN:C	2.61	0.43
1:A:145:GLN:N	1:A:145:GLN:HE21	2.16	0.43
1:C:420:GLU:O	1:C:423:HIS:N	2.52	0.43
1:C:463:LYS:O	1:C:467:LYS:HB2	2.19	0.43
2:H:1508:ILE:HD12	2:H:1508:ILE:HA	1.83	0.43
1:A:95:GLU:OE2	1:A:97:LEU:HD21	2.19	0.43
1:C:439:ILE:O	1:C:443:LEU:HB2	2.17	0.43
1:D:650:ARG:O	1:D:654:MET:HB2	2.19	0.43
2:E:1213:SER:O	2:E:1216:ARG:N	2.52	0.43
2:F:1016:ARG:NH1	2:F:1034:ALA:HA	2.34	0.43
2:F:1016:ARG:NH1	2:F:1034:ALA:HB2	2.33	0.43
2:G:1647:ARG:CZ	2:G:1673:ASP:CG	2.92	0.43
1:B:281:LEU:CD2	1:B:294:TYR:OH	2.66	0.43
2:G:1620:ASN:ND2	2:G:1632:GLN:NE2	2.67	0.43
1:D:653:GLU:O	1:D:656:GLU:N	2.52	0.42
2:E:1263:ILE:HD13	2:E:1263:ILE:HA	1.90	0.42
2:G:1628:TYR:OH	2:G:1719:LEU:HG	2.19	0.42
2:G:1668:ARG:O	2:G:1671:VAL:HB	2.19	0.42
2:G:1705:PRO:O	2:G:1706:PHE:O	2.37	0.42
1:A:128:GLU:OE1	2:E:1238:GLN:HG2	2.19	0.42
1:B:294:TYR:O	1:B:294:TYR:CD1	2.72	0.42
1:B:331:ASN:HB3	1:B:352:PHE:CE1	2.54	0.42
2:E:1220:ASN:ND2	2:E:1230:THR:OG1	2.52	0.42
2:E:1253:LEU:CD1	2:E:1265:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:HIS:ND1	1:C:542:PRO:HD2	2.35	0.42
1:D:703:LEU:HD22	1:D:746:LEU:CD1	2.47	0.42
1:C:489:TYR:HB2	1:C:490:MET:H	1.56	0.42
1:C:572:ASP:O	1:C:573:VAL:HG22	2.18	0.42
2:E:1235:ASN:OD1	2:E:1238:GLN:HG3	2.20	0.42
2:G:1662:GLY:O	2:G:1665:ILE:HG22	2.19	0.42
2:G:1688:ASP:OD1	2:G:1688:ASP:N	2.51	0.42
2:H:1410:ASP:OD1	2:H:1412:GLN:HB2	2.19	0.42
2:H:1450:LEU:HD11	2:H:1479:ILE:HG13	2.01	0.42
1:A:31:ASP:O	1:A:35:LYS:HG3	2.20	0.42
1:B:308:GLN:CA	1:B:308:GLN:HE21	2.33	0.42
1:C:438:LEU:O	1:C:439:ILE:C	2.62	0.42
2:G:1616:ARG:HG2	2:G:1616:ARG:HH11	1.84	0.42
2:G:1687:LEU:HA	2:G:1690:ILE:CB	2.19	0.42
1:B:267:LYS:HD3	1:B:296:VAL:HB	2.02	0.42
1:C:448:TYR:O	1:C:451:VAL:HB	2.19	0.42
1:D:727:ARG:O	2:H:1437:LEU:HD13	2.20	0.42
1:C:471:LEU:HA	1:C:501:LYS:O	2.19	0.42
1:D:702:ASP:OD2	1:D:704:SER:HB3	2.19	0.42
2:G:1664:GLU:C	2:G:1666:LEU:H	2.27	0.42
2:H:1483:ALA:HB3	2:H:1486:GLU:HB2	2.02	0.42
2:H:1500:THR:OG1	2:H:1501:HIS:N	2.52	0.42
1:A:127:ARG:NH1	1:A:127:ARG:CG	2.78	0.42
1:C:514:MET:CE	1:C:548:LEU:HD13	2.33	0.42
1:C:567:GLN:HG2	1:C:568:ASN:N	2.34	0.42
1:D:682:THR:HA	1:D:685:TRP:CE3	2.55	0.42
2:E:1210:ASP:OD2	2:E:1304:LYS:NZ	2.49	0.42
2:E:1222:VAL:O	2:E:1225:LYS:HB2	2.19	0.42
2:G:1686:GLU:C	2:G:1690:ILE:HD12	2.44	0.42
1:C:467:LYS:HD3	1:C:496:VAL:HB	2.01	0.42
1:D:700:ILE:CD1	1:D:700:ILE:N	2.83	0.42
1:D:708:GLN:O	1:D:712:LYS:CE	2.67	0.42
2:G:1713:ASP:HA	2:G:1716:LYS:HB2	2.00	0.42
1:B:345:GLN:HE21	1:B:345:GLN:HB2	1.71	0.42
1:D:690:MET:HE3	1:D:733:LEU:CB	2.50	0.42
2:E:1316:LYS:C	2:E:1318:TYR:H	2.28	0.42
2:F:1107:ASP:C	2:F:1109:ASP:N	2.78	0.42
2:H:1477:ARG:NH1	2:H:1520:PRO:CB	2.79	0.42
1:C:533:LEU:HD22	1:C:533:LEU:C	2.45	0.41
1:C:582:SER:HB2	1:C:583:HIS:ND1	2.34	0.41
1:D:717:LEU:O	1:D:720:LEU:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1065:ILE:O	2:F:1069:MET:HB2	2.20	0.41
1:C:446:GLN:C	1:C:448:TYR:H	2.27	0.41
2:H:1477:ARG:H	2:H:1477:ARG:HG2	1.27	0.41
1:C:440:LYS:NZ	2:G:1705:PRO:HB2	2.35	0.41
1:C:572:ASP:O	1:C:573:VAL:O	2.38	0.41
1:D:621:LEU:HD11	1:D:625:LEU:HD11	2.01	0.41
1:D:637:GLN:HB2	2:H:1505:PRO:HB3	2.00	0.41
2:E:1205:LYS:HB2	2:E:1248:PRO:HA	2.02	0.41
2:E:1239:ALA:O	2:E:1240:LEU:C	2.63	0.41
2:E:1261:ASP:CB	2:E:1264:GLU:HB2	2.50	0.41
2:F:1077:ARG:HH11	2:F:1077:ARG:CG	2.33	0.41
2:G:1687:LEU:HD13	2:G:1687:LEU:N	2.32	0.41
1:A:132:HIS:HE1	1:A:134:THR:OG1	2.02	0.41
1:B:231:ASP:O	1:B:235:LYS:HG3	2.19	0.41
1:B:243:LEU:HD12	1:B:243:LEU:HA	1.92	0.41
1:C:490:MET:H	1:C:490:MET:HG2	1.70	0.41
1:D:660:ILE:C	1:D:662:ALA:N	2.76	0.41
2:E:1219:LEU:O	2:E:1222:VAL:HB	2.20	0.41
2:E:1284:TYR:CD2	2:E:1284:TYR:C	2.98	0.41
2:G:1650:LEU:CD2	2:G:1651:VAL:N	2.83	0.41
1:A:141:HIS:CD2	1:A:144:ARG:HG2	2.56	0.41
1:B:242:ASN:OD1	2:F:1018:LEU:HD13	2.21	0.41
1:B:364:ASP:O	1:B:368:ASN:N	2.54	0.41
1:C:478:PHE:CD1	1:C:478:PHE:C	2.98	0.41
1:C:566:ARG:HG2	1:C:566:ARG:NH1	2.36	0.41
2:F:1035:ASN:O	2:F:1036:GLY:C	2.63	0.41
2:F:1055:MET:CB	2:F:1089:MET:HE2	2.40	0.41
2:G:1647:ARG:NH1	2:G:1673:ASP:OD2	2.53	0.41
2:G:1679:ILE:HG23	2:G:1701:HIS:CA	2.51	0.41
1:C:438:LEU:HD21	2:G:1615:ILE:HG13	2.02	0.41
1:D:624:LEU:O	1:D:627:HIS:HB2	2.21	0.41
1:A:173:VAL:O	1:A:173:VAL:HG23	2.20	0.41
1:C:420:GLU:O	1:C:422:ILE:N	2.53	0.41
1:D:693:GLU:CG	1:D:732:HIS:HE1	2.34	0.41
1:D:721:PHE:O	1:D:725:VAL:HG13	2.19	0.41
2:G:1719:LEU:HA	2:G:1719:LEU:HD13	1.86	0.41
2:H:1407:LEU:HD12	2:H:1431:PHE:O	2.20	0.41
2:H:1412:GLN:HE21	2:H:1412:GLN:HB3	1.65	0.41
1:A:146:LEU:O	1:A:191:LEU:N	2.52	0.41
1:B:358:ASP:C	1:B:360:SER:N	2.78	0.41
1:C:544:ARG:HE	1:C:592:ASP:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1240:LEU:O	2:E:1243:VAL:N	2.53	0.41
1:B:267:LYS:HE2	1:B:299:GLU:CG	2.47	0.41
1:B:268:LEU:HA	1:B:271:LEU:CD1	2.48	0.41
1:B:374:ASP:O	1:B:376:MET:HG3	2.21	0.41
1:C:458:MET:HA	1:C:461:ASP:OD2	2.20	0.41
1:C:488:HIS:O	1:C:489:TYR:CD1	2.74	0.41
1:C:582:SER:HB2	1:C:583:HIS:CE1	2.55	0.41
2:F:1026:GLU:HG3	2:F:1112:ARG:CD	2.49	0.41
2:F:1039:ALA:O	2:F:1043:VAL:HG23	2.20	0.41
2:G:1707:ASP:O	2:G:1708:ILE:C	2.63	0.41
2:H:1420:ASN:HD21	2:H:1432:GLN:HE21	1.64	0.41
1:A:55:ILE:HD13	1:B:240:LYS:HB2	2.02	0.41
1:A:66:SER:O	1:A:67:LYS:C	2.64	0.41
1:C:526:SER:C	1:C:528:GLU:N	2.76	0.41
2:F:1050:LEU:HD12	2:F:1077:ARG:HB3	2.02	0.41
2:G:1652:LEU:HD12	2:G:1679:ILE:HB	2.03	0.41
2:G:1687:LEU:C	2:G:1690:ILE:H	2.29	0.41
2:H:1409:VAL:O	2:H:1454:ASP:HB3	2.21	0.41
1:A:36:LEU:O	1:A:40:LYS:HG2	2.21	0.40
1:A:138:GLN:CD	1:A:147:ILE:HD11	2.46	0.40
1:B:272:LYS:HD2	1:B:302:ASP:CG	2.47	0.40
1:C:493:GLU:HB2	1:C:532:HIS:CE1	2.56	0.40
2:E:1280:ILE:O	2:E:1301:HIS:HA	2.22	0.40
2:F:1077:ARG:HE	2:F:1120:PRO:HG2	1.83	0.40
1:A:93:GLU:HG3	1:A:132:HIS:NE2	2.36	0.40
1:D:671:LEU:CD2	1:D:700:ILE:HA	2.52	0.40
1:B:247:LYS:NZ	2:G:1629:GLN:HE22	2.19	0.40
1:D:737:LEU:HD22	1:D:746:LEU:HD22	1.96	0.40
1:D:741:HIS:HB3	1:D:744:ARG:O	2.20	0.40
2:F:1019:LEU:O	2:F:1023:PHE:CD2	2.74	0.40
1:C:430:HIS:O	1:C:431:ASP:C	2.63	0.40
1:C:545:GLN:HB2	1:C:592:ASP:O	2.21	0.40
1:C:560:SER:C	1:C:562:PHE:N	2.79	0.40
2:E:1205:LYS:HD2	2:E:1246:GLU:O	2.21	0.40
2:G:1660:MET:HE3	2:G:1665:ILE:CD1	2.48	0.40
2:G:1664:GLU:C	2:G:1666:LEU:N	2.77	0.40
1:A:55:ILE:O	1:A:58:MET:HB2	2.22	0.40
1:B:242:ASN:O	1:B:247:LYS:HB2	2.22	0.40
1:B:313:LEU:HD21	1:B:389:ILE:HD13	2.03	0.40
2:E:1212:GLN:HE21	2:E:1212:GLN:HB2	1.48	0.40
2:F:1007:LEU:HD12	2:F:1031:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1070:LYS:HG2	2:F:1076:ILE:HG21	2.01	0.40
2:G:1653:LEU:HG	2:G:1654:ASP:N	2.36	0.40
2:H:1440:LEU:HD12	2:H:1472:ILE:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:ASP:O	2:E:1294:LYS:NZ[4_565]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	7	32
1	B	180/182 (99%)	148 (82%)	24 (13%)	8 (4%)	2	12
1	C	179/182 (98%)	139 (78%)	23 (13%)	17 (10%)	0	2
1	D	180/182 (99%)	145 (81%)	27 (15%)	8 (4%)	2	12
2	E	117/119 (98%)	94 (80%)	19 (16%)	4 (3%)	3	17
2	F	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	4	23
2	G	117/119 (98%)	79 (68%)	26 (22%)	12 (10%)	0	2
2	H	117/119 (98%)	89 (76%)	15 (13%)	13 (11%)	0	1
All	All	1186/1204 (98%)	949 (80%)	169 (14%)	68 (6%)	1	8

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	168	ASN

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Mol	Chain	Res	Type
1	B	248	TYR
1	B	300	ILE
1	B	307	ASP
1	B	344	ARG
1	B	364	ASP
1	B	371	GLU
1	C	413	SER
1	C	415	THR
1	C	489	TYR
1	C	499	GLU
1	C	545	GLN
1	C	568	ASN
1	C	575	ILE
1	D	615	THR
1	D	683	PHE
1	D	700	ILE
2	F	1092	GLU
2	G	1613	SER
2	G	1614	GLY
2	G	1699	LEU
2	G	1701	HIS
2	G	1708	ILE
2	H	1428	TYR
2	H	1460	MET
2	H	1487	LEU
2	H	1499	LEU
2	H	1508	ILE
1	B	308	GLN
1	B	343	ASP
1	C	446	GLN
1	C	498	GLY
1	C	572	ASP
1	D	654	MET
1	D	707	ASP
1	D	771	GLU
2	E	1310	GLU
2	F	1108	ILE
2	G	1650	LEU
2	G	1706	PHE
2	G	1709	ASP
2	H	1446	GLU
2	H	1514	ALA

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Mol	Chain	Res	Type
2	H	1518	TYR
1	A	171	GLU
1	C	542	PRO
1	D	763	ASP
2	E	1233	ALA
2	F	1021	GLU
2	H	1467	LYS
1	C	487	THR
1	C	507	ASP
1	C	573	VAL
2	E	1309	ASP
2	H	1462	GLY
2	H	1496	LEU
1	C	421	LEU
1	D	684	ASN
2	G	1716	LYS
2	H	1448	PRO
1	C	418	THR
2	E	1214	GLY
2	G	1691	GLN
2	G	1690	ILE
2	H	1520	PRO
1	C	451	VAL
2	G	1720	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/167 (98%)	150 (92%)	14 (8%)	10	36
1	B	167/167 (100%)	145 (87%)	22 (13%)	4	18
1	C	161/167 (96%)	122 (76%)	39 (24%)	1	4
1	D	165/167 (99%)	150 (91%)	15 (9%)	9	33
2	E	102/105 (97%)	87 (85%)	15 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	105/105 (100%)	81 (77%)	24 (23%)	1	5
2	G	104/105 (99%)	84 (81%)	20 (19%)	1	8
2	H	102/105 (97%)	85 (83%)	17 (17%)	2	12
All	All	1070/1088 (98%)	904 (84%)	166 (16%)	2	13

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	50	ARG
1	A	72	LYS
1	A	126	SER
1	A	133	LEU
1	A	145	GLN
1	A	146	LEU
1	A	147	ILE
1	A	148	LEU
1	A	151	ASP
1	A	165	ILE
1	A	167	GLN
1	A	180	ILE
1	A	191	LEU
1	B	213	SER
1	B	214	ASP
1	B	215	THR
1	B	218	THR
1	B	228	SER
1	B	234	ASN
1	B	249	ASP
1	B	299	GLU
1	B	328	GLU
1	B	337	LEU
1	B	345	GLN
1	B	348	LEU
1	B	360	SER
1	B	364	ASP
1	B	365	ILE
1	B	371	GLU
1	B	372	ASP
1	B	373	VAL
1	B	375	ILE

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Mol	Chain	Res	Type
1	B	384	GLU
1	B	386	LEU
1	B	391	LEU
1	C	415	THR
1	C	417	LEU
1	C	418	THR
1	C	419	ASN
1	C	429	ARG
1	C	434	ASN
1	C	440	LYS
1	C	443	LEU
1	C	450	ARG
1	C	455	ILE
1	C	466	SER
1	C	469	SER
1	C	472	LYS
1	C	473	THR
1	C	484	ASN
1	C	488	HIS
1	C	489	TYR
1	C	491	THR
1	C	496	VAL
1	C	500	ILE
1	C	502	ASP
1	C	504	SER
1	C	512	LYS
1	C	515	ARG
1	C	528	GLU
1	C	533	LEU
1	C	536	SER
1	C	540	ASP
1	C	545	GLN
1	C	547	ILE
1	C	548	LEU
1	C	551	ASP
1	C	564	ASP
1	C	566	ARG
1	C	571	GLU
1	C	573	VAL
1	C	575	ILE
1	C	581	THR
1	C	583	HIS

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Mol	Chain	Res	Type
1	D	617	LEU
1	D	618	THR
1	D	638	LEU
1	D	642	ASN
1	D	656	GLU
1	D	672	LYS
1	D	700	ILE
1	D	720	LEU
1	D	726	SER
1	D	736	SER
1	D	737	LEU
1	D	745	GLN
1	D	765	ILE
1	D	773	VAL
1	D	780	ILE
2	E	1204	GLU
2	E	1212	GLN
2	E	1213	SER
2	E	1220	ASN
2	E	1224	ASN
2	E	1240	LEU
2	E	1252	LEU
2	E	1260	MET
2	E	1263	ILE
2	E	1266	LEU
2	E	1269	MET
2	E	1271	VAL
2	E	1275	ASN
2	E	1276	ILE
2	E	1286	GLU
2	F	1012	GLN
2	F	1016	ARG
2	F	1020	ASN
2	F	1025	LYS
2	F	1040	LEU
2	F	1047	ARG
2	F	1052	LEU
2	F	1063	ILE
2	F	1065	ILE
2	F	1066	LEU
2	F	1068	ARG
2	F	1069	MET

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Mol	Chain	Res	Type
2	F	1070	LYS
2	F	1071	VAL
2	F	1074	GLU
2	F	1086	GLU
2	F	1087	LEU
2	F	1099	LEU
2	F	1107	ASP
2	F	1108	ILE
2	F	1109	ASP
2	F	1111	ILE
2	F	1113	ASP
2	F	1119	LEU
2	G	1621	GLU
2	G	1622	VAL
2	G	1625	LYS
2	G	1638	GLN
2	G	1647	ARG
2	G	1649	ASP
2	G	1650	LEU
2	G	1653	LEU
2	G	1660	MET
2	G	1674	GLU
2	G	1680	ILE
2	G	1687	LEU
2	G	1689	MET
2	G	1691	GLN
2	G	1692	GLU
2	G	1702	PHE
2	G	1704	LYS
2	G	1706	PHE
2	G	1709	ASP
2	G	1719	LEU
2	H	1412	GLN
2	H	1415	ILE
2	H	1440	LEU
2	H	1443	VAL
2	H	1444	THR
2	H	1457	ILE
2	H	1460	MET
2	H	1461	ASP
2	H	1465	ILE
2	H	1466	LEU

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Mol	Chain	Res	Type
2	H	1468	ARG
2	H	1476	ILE
2	H	1477	ARG
2	H	1482	THR
2	H	1499	LEU
2	H	1508	ILE
2	H	1511	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	42	ASN
1	A	75	HIS
1	A	119	HIS
1	A	141	HIS
1	A	145	GLN
1	A	168	ASN
1	B	223	HIS
1	B	237	GLN
1	B	288	HIS
1	B	308	GLN
1	B	332	HIS
1	B	341	HIS
1	B	345	GLN
1	C	541	HIS
1	C	553	HIS
1	D	627	HIS
1	D	637	GLN
1	D	642	ASN
1	D	646	GLN
1	D	670	ASN
1	D	688	HIS
1	D	708	GLN
1	D	723	GLN
1	D	732	HIS
2	E	1212	GLN
2	E	1224	ASN
2	E	1238	GLN
2	E	1275	ASN
2	E	1291	GLN
2	F	1020	ASN

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Mol	Chain	Res	Type
2	F	1024	ASN
2	F	1038	GLN
2	F	1075	ASN
2	F	1091	GLN
2	G	1612	GLN
2	G	1629	GLN
2	G	1632	GLN
2	G	1638	GLN
2	G	1691	GLN
2	H	1412	GLN
2	H	1424	ASN
2	H	1432	GLN
2	H	1438	GLN
2	H	1475	ASN
2	H	1491	GLN
2	H	1501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.