



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:25 AM UTC

PDB ID : 1G8X / pdb_00001g8x
Title : STRUCTURE OF A GENETICALLY ENGINEERED MOLECULAR MOTOR
Authors : Kliche, W.; Fujita-Becker, S.; Kollmar, M.; Manstein, D.J.; Kull, F.J.
Deposited on : 2000-11-21
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

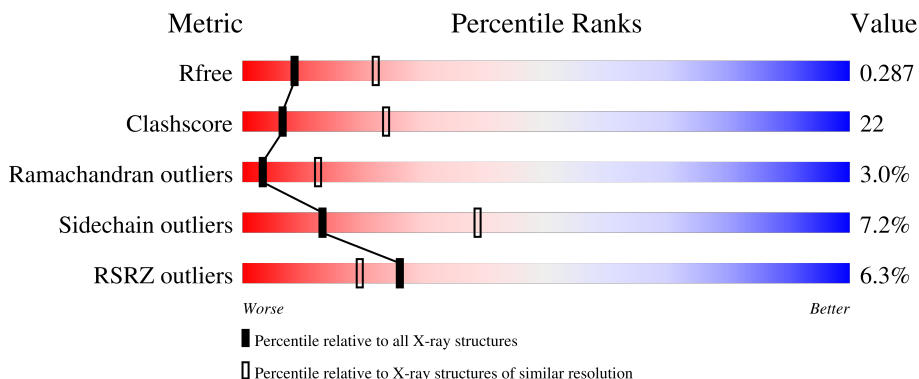
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

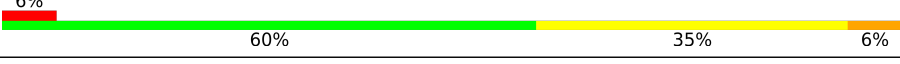
The reported resolution of this entry is 2.80 Å.

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1010	
1	B	1010	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16292 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 MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1009	Total	C	N	O	S	0	0	0
			8111	5131	1406	1556	18			
1	B	1009	Total	C	N	O	S	0	0	0
			8111	5131	1406	1556	18			

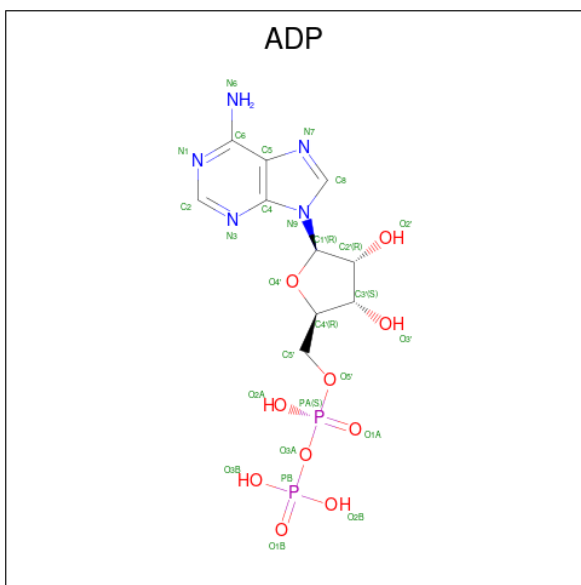
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ARG	engineered mutation	UNP P08799
A	312	CYS	TYR	engineered mutation	UNP P08799
A	321	GLU	SER	engineered mutation	UNP P08799
A	443	SER	GLN	engineered mutation	UNP P08799
A	489	VAL	LEU	engineered mutation	UNP P08799
B	238	GLU	ARG	engineered mutation	UNP P08799
B	312	CYS	TYR	engineered mutation	UNP P08799
B	321	GLU	SER	engineered mutation	UNP P08799
B	443	SER	GLN	engineered mutation	UNP P08799
B	489	VAL	LEU	engineered mutation	UNP P08799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

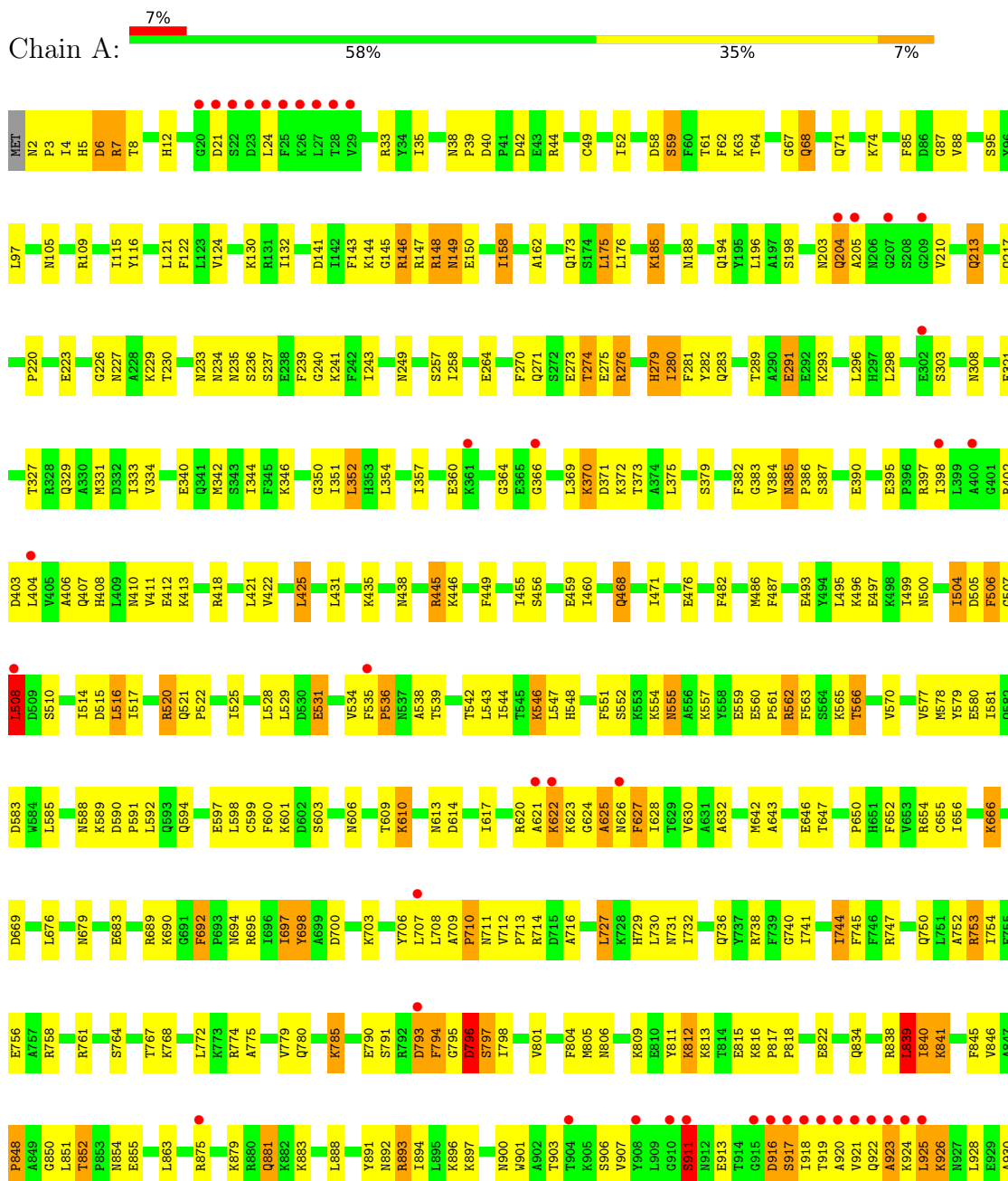
- Molecule 4 is water.

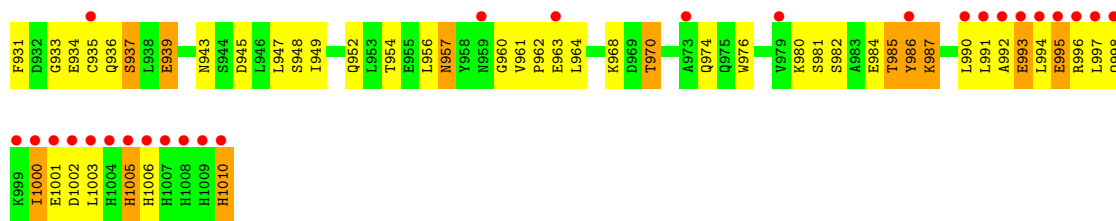
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	7	Total O 7 7	0	0

3 Residue-property plots

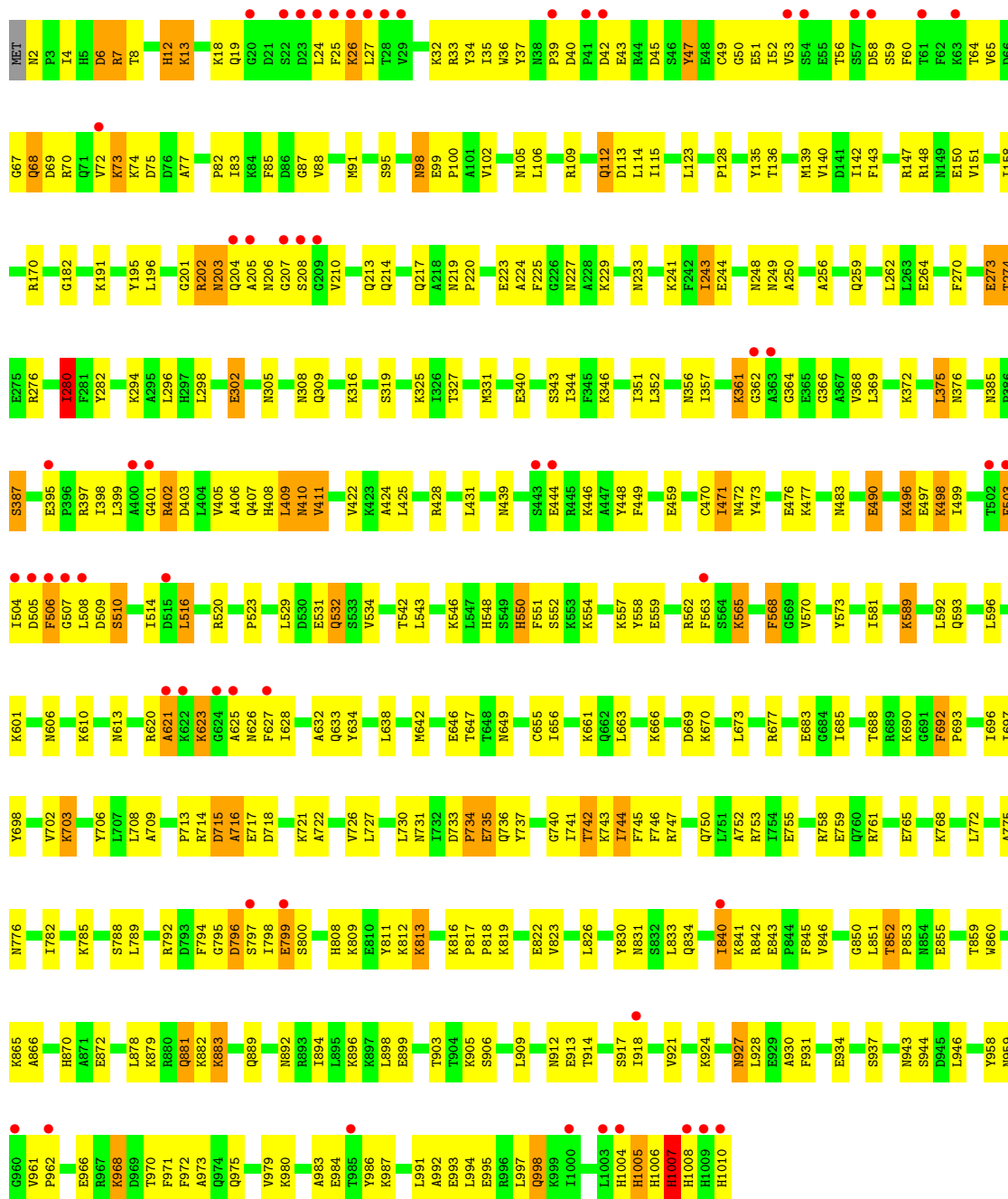
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3





• Molecule 1: MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.42Å 155.42Å 143.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.15 – 2.80 41.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.15-2.80) 97.6 (41.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.290 0.231 , 0.287	Depositor DCC
R_{free} test set	5996 reflections (8.18%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16292	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.55	4/8267 (0.0%)	0.99	50/11157 (0.4%)
1	B	0.49	1/8267 (0.0%)	0.96	26/11157 (0.2%)
All	All	0.52	5/16534 (0.0%)	0.97	76/22314 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	LYS	C-N	-15.11	1.14	1.33
1	A	445	ARG	C-N	9.37	1.45	1.33
1	B	796	ASP	N-CA	6.20	1.54	1.46
1	A	911	SER	CA-C	-5.68	1.45	1.52
1	A	506	PHE	N-CA	5.19	1.52	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	496	LYS	N-CA-C	-11.11	95.87	110.53
1	B	796	ASP	N-CA-C	10.36	127.72	114.56
1	A	911	SER	N-CA-C	-9.20	91.20	110.80
1	B	649	ASN	N-CA-C	-8.49	99.11	109.72
1	A	796	ASP	CA-CB-CG	-8.37	104.23	112.60
1	A	796	ASP	CB-CA-C	-7.98	94.54	110.42
1	A	995	GLU	N-CA-C	-7.68	102.84	112.90
1	A	446	LYS	O-C-N	-7.50	114.88	123.42
1	B	735	GLU	N-CA-C	-7.28	104.55	113.50
1	A	926	LYS	N-CA-C	-7.18	104.52	113.28
1	A	930	ALA	N-CA-C	-7.17	104.69	113.50
1	A	692	PHE	CA-C-N	7.00	126.98	119.28
1	A	692	PHE	C-N-CA	7.00	126.98	119.28
1	B	796	ASP	CB-CA-C	-6.84	98.46	109.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	936	GLN	N-CA-C	-6.83	104.25	114.64
1	A	796	ASP	N-CA-C	6.81	125.31	110.80
1	A	445	ARG	O-C-N	-6.77	114.43	123.23
1	A	993	GLU	N-CA-C	-6.72	105.07	113.20
1	A	991	LEU	N-CA-C	-6.58	104.85	114.39
1	B	498	LYS	N-CA-C	6.50	120.21	111.24
1	A	506	PHE	N-CA-C	6.46	124.57	110.80
1	A	279	HIS	N-CA-C	6.45	118.85	111.11
1	A	1000	ILE	N-CA-C	-6.35	106.54	112.83
1	B	883	LYS	N-CA-C	-6.25	104.58	111.82
1	A	1003	LEU	N-CA-C	-6.24	104.93	112.54
1	B	510	SER	N-CA-C	-6.12	104.72	111.82
1	B	143	PHE	N-CA-C	6.08	120.70	113.28
1	A	583	ASP	N-CA-C	6.06	120.47	113.38
1	A	1005	HIS	N-CA-C	-6.04	105.72	114.12
1	B	623	LYS	N-CA-C	-6.01	105.80	113.01
1	B	930	ALA	N-CA-C	-5.97	105.48	112.89
1	B	692	PHE	CA-C-N	5.88	127.19	119.84
1	B	692	PHE	C-N-CA	5.88	127.19	119.84
1	A	198	SER	N-CA-C	5.82	117.43	111.14
1	B	758	ARG	N-CA-C	-5.80	104.95	111.28
1	B	112	GLN	N-CA-C	-5.77	105.55	112.59
1	B	998	GLN	N-CA-C	-5.77	105.74	112.89
1	B	1007	HIS	N-CA-C	-5.71	106.17	113.01
1	A	122	PHE	N-CA-C	5.67	118.67	110.28
1	A	939	GLU	N-CA-C	-5.66	104.38	112.13
1	A	669	ASP	N-CA-C	5.58	117.81	111.11
1	A	839	LEU	N-CA-C	-5.57	98.93	110.80
1	A	303	SER	N-CA-C	5.55	119.58	112.26
1	A	476	GLU	N-CA-C	-5.55	105.31	111.36
1	A	986	TYR	N-CA-C	-5.52	108.33	114.62
1	A	937	SER	N-CA-C	-5.46	106.67	113.55
1	A	308	ASN	N-CA-C	5.46	117.01	109.54
1	A	210	VAL	N-CA-C	-5.42	104.97	112.50
1	A	194	GLN	N-CA-C	-5.42	105.29	111.14
1	A	711	ASN	N-CA-C	5.40	117.79	110.88
1	B	717	GLU	N-CA-C	-5.36	105.54	111.71
1	A	385	ASN	CA-C-N	5.35	125.67	119.47
1	A	385	ASN	C-N-CA	5.35	125.67	119.47
1	B	280	ILE	CB-CA-C	-5.35	105.04	112.04
1	B	927	ASN	N-CA-C	-5.30	105.91	112.38
1	A	650	PRO	N-CA-C	5.29	119.35	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	LEU	N-CA-C	5.24	118.47	111.24
1	A	551	PHE	N-CA-C	5.23	120.02	113.43
1	B	647	THR	N-CA-C	-5.22	104.51	111.87
1	A	535	PHE	CA-C-N	5.20	126.34	119.84
1	A	535	PHE	C-N-CA	5.20	126.34	119.84
1	A	62	PHE	N-CA-C	5.20	117.57	109.52
1	A	522	PRO	CA-C-N	5.15	124.91	119.76
1	A	522	PRO	C-N-CA	5.15	124.91	119.76
1	B	750	GLN	N-CA-C	5.14	116.69	111.14
1	B	1005	HIS	N-CA-C	-5.14	106.70	112.87
1	B	47	TYR	N-CA-C	5.12	117.45	109.52
1	A	906	SER	N-CA-C	-5.10	107.01	113.18
1	B	906	SER	N-CA-C	-5.08	107.47	113.97
1	A	852	THR	N-CA-C	-5.07	103.29	110.29
1	A	652	PHE	N-CA-C	5.06	116.98	108.73
1	A	996	ARG	N-CA-C	-5.05	106.87	112.57
1	A	446	LYS	CA-C-N	5.03	127.47	120.63
1	A	446	LYS	C-N-CA	5.03	127.47	120.63
1	A	709	ALA	CA-C-N	5.02	126.11	119.84
1	A	709	ALA	C-N-CA	5.02	126.11	119.84

There are no chirality outliers.

There are no planarity outliers.

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	8111	0	8037	360	0
1	B	8111	0	8038	345	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	2	0
4	A	7	0	0	1	0
4	B	7	0	0	1	0
All	All	16292	0	16099	704	0

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 22.

All (704) 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)
1:B:834:GLN:HE22	1:B:845:PHE:HB3	1.17	1.05
1:A:697:ILE:HD13	1:A:697:ILE:H	1.19	1.04
1:B:532:GLN:OE1	1:B:542:THR:HG22	1.66	0.95
1:A:623:LYS:HE3	1:A:626:ASN:H	1.31	0.95
1:B:543:LEU:HD23	1:B:581:ILE:HD11	1.48	0.94
1:A:848:PRO:HB2	1:A:851:LEU:HD23	1.50	0.92
1:A:2:ASN:HD21	1:A:5:HIS:HD2	1.14	0.90
1:B:509:ASP:HB2	1:B:557:LYS:HZ3	1.36	0.90
1:B:918:ILE:HG13	1:B:997:LEU:HD22	1.55	0.89
1:A:233:ASN:ND2	1:A:235:ASN:H	1.70	0.88
1:A:561:PRO:HB3	1:A:578:MET:HE1	1.53	0.88
1:B:796:ASP:O	1:B:881:GLN:OE1	1.93	0.86
1:B:797:SER:OG	1:B:799:GLU:OE1	1.93	0.86
1:A:273:GLU:O	1:A:274:THR:HB	1.73	0.86
1:A:817:PRO:HB2	1:A:818:PRO:HD3	1.58	0.85
1:A:931:PHE:O	1:A:934:GLU:HG2	1.76	0.85
1:B:35:ILE:HD11	1:B:77:ALA:HB1	1.59	0.84
1:A:2:ASN:HD21	1:A:5:HIS:CD2	1.95	0.84
1:A:925:LEU:HD21	1:A:990:LEU:HB3	1.60	0.84
1:B:703:LYS:HE2	1:B:703:LYS:O	1.79	0.83
1:A:520:ARG:HG3	1:A:521:GLN:HG2	1.61	0.83
1:A:986:TYR:O	1:A:990:LEU:HB2	1.79	0.83
1:A:68:GLN:H	1:A:68:GLN:HE21	1.26	0.83
1:A:543:LEU:HD23	1:A:581:ILE:HD11	1.60	0.83
1:B:509:ASP:HB2	1:B:557:LYS:NZ	1.93	0.82
1:B:601:LYS:HG2	1:B:613:ASN:ND2	1.94	0.82
1:B:809:LYS:O	1:B:813:LYS:HD3	1.80	0.81
1:B:139:MET:HE2	1:B:139:MET:HA	1.63	0.81
1:B:225:PHE:HA	1:B:280:ILE:HD11	1.62	0.81
1:A:622:LYS:HE2	1:A:624:GLY:H	1.43	0.80
1:A:697:ILE:H	1:A:697:ILE:CD1	1.94	0.79
1:A:907:VAL:O	1:A:911:SER:HB3	1.82	0.79
1:B:302:GLU:HA	1:B:308:ASN:HB3	1.63	0.78
1:A:455:ILE:HD12	1:A:456:SER:H	1.49	0.78
1:A:539:THR:O	1:A:542:THR:HG22	1.83	0.78
1:B:655:CYS:C	1:B:656:ILE:HD12	2.09	0.77
1:B:834:GLN:NE2	1:B:845:PHE:HB3	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASN:ND2	1:A:557:LYS:H	1.81	0.76
1:A:697:ILE:HD13	1:A:697:ILE:N	2.00	0.76
1:A:839:LEU:C	1:A:841:LYS:H	1.94	0.76
1:A:654:ARG:HD2	1:A:679:ASN:HB2	1.66	0.76
1:A:68:GLN:H	1:A:68:GLN:NE2	1.83	0.76
1:A:371:ASP:C	1:A:372:LYS:HD2	2.11	0.76
1:A:666:LYS:HE2	1:A:666:LYS:HA	1.66	0.75
1:B:68:GLN:NE2	1:B:70:ARG:HH21	1.85	0.75
1:A:516:LEU:HD22	1:A:516:LEU:O	1.87	0.74
1:A:839:LEU:O	1:A:841:LYS:N	2.21	0.73
1:A:233:ASN:HD22	1:A:234:ASN:N	1.87	0.73
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.70	0.73
1:A:628:ILE:HG13	1:A:632:ALA:HB3	1.70	0.72
1:B:499:ILE:HD11	1:B:740:GLY:HA2	1.70	0.72
1:A:493:GLU:HG2	1:A:695:ARG:HH12	1.52	0.72
1:A:147:ARG:HD3	1:A:150:GLU:OE1	1.90	0.72
1:A:555:ASN:HD22	1:A:557:LYS:H	1.37	0.72
1:A:753:ARG:HG2	1:A:753:ARG:HH11	1.53	0.71
1:A:274:THR:CG2	1:A:274:THR:O	2.38	0.71
1:B:508:LEU:HD13	1:B:508:LEU:O	1.91	0.71
1:A:520:ARG:HH11	1:A:520:ARG:HA	1.54	0.70
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.73	0.70
1:B:797:SER:OG	1:B:799:GLU:CD	2.34	0.70
1:A:589:LYS:O	1:A:589:LYS:HD3	1.91	0.70
1:B:13:LYS:HE3	1:B:13:LYS:HA	1.74	0.70
1:A:342:MET:HG3	1:A:346:LYS:HZ3	1.57	0.70
1:A:141:ASP:HA	1:A:144:LYS:HE2	1.72	0.69
1:A:774:ARG:HH21	1:A:822:GLU:CD	2.00	0.69
1:A:809:LYS:O	1:A:813:LYS:HD3	1.92	0.69
1:A:610:LYS:HZ3	1:A:610:LYS:HB2	1.57	0.69
1:A:925:LEU:HD11	1:A:990:LEU:HD13	1.74	0.69
1:B:224:ALA:O	1:B:280:ILE:HG13	1.92	0.69
1:B:532:GLN:HE21	1:B:532:GLN:HA	1.56	0.69
1:B:782:ILE:HG21	1:B:859:THR:HG22	1.75	0.69
1:B:401:GLY:C	1:B:402:ARG:HD3	2.18	0.69
1:B:496:LYS:C	1:B:498:LYS:H	2.00	0.69
1:B:1007:HIS:HA	1:B:1010:HIS:CD2	2.28	0.69
1:A:58:ASP:HA	1:A:74:LYS:HD2	1.74	0.68
1:A:706:TYR:HB2	1:A:712:VAL:HG23	1.76	0.68
1:B:918:ILE:HD11	1:B:998:GLN:HA	1.74	0.68
1:B:817:PRO:HB2	1:B:818:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LYS:HD2	1:B:243:ILE:HD11	1.76	0.68
1:A:811:TYR:O	1:A:811:TYR:CD2	2.46	0.68
1:A:848:PRO:HB2	1:A:851:LEU:CD2	2.24	0.68
1:B:273:GLU:O	1:B:274:THR:HB	1.93	0.67
1:A:340:GLU:O	1:A:344:ILE:HG13	1.93	0.67
1:B:621:ALA:O	1:B:628:ILE:HD13	1.93	0.67
1:B:795:GLY:HA3	1:B:800:SER:OG	1.95	0.67
1:A:793:ASP:CG	1:A:794:PHE:N	2.52	0.67
1:A:708:LEU:HD13	1:A:730:LEU:HD11	1.77	0.67
1:A:922:GLN:HB2	1:A:994:LEU:HD11	1.77	0.66
1:B:25:PHE:O	1:B:26:LYS:HG3	1.96	0.66
1:B:385:ASN:HB3	1:B:387:SER:OG	1.95	0.66
1:B:497:GLU:OE1	1:B:742:THR:HG22	1.95	0.66
1:A:918:ILE:HG23	1:A:922:GLN:HE21	1.59	0.66
1:A:921:VAL:HG12	1:A:994:LEU:HD21	1.77	0.66
1:B:202:ARG:O	1:B:203:ASN:C	2.39	0.66
1:A:121:LEU:HD11	1:A:486:MET:HA	1.78	0.66
1:A:342:MET:HG3	1:A:346:LYS:NZ	2.10	0.66
1:A:620:ARG:HB3	1:A:628:ILE:HG22	1.77	0.66
1:A:628:ILE:HD11	1:A:632:ALA:HB1	1.78	0.66
1:B:768:LYS:O	1:B:772:LEU:HD13	1.95	0.66
1:B:399:LEU:HD12	1:B:403:ASP:O	1.97	0.65
1:B:504:ILE:HD11	1:B:690:LYS:HZ2	1.62	0.65
1:B:361:LYS:HE3	1:B:361:LYS:HA	1.78	0.65
1:B:623:LYS:NZ	1:B:625:ALA:HB3	2.12	0.65
1:A:797:SER:O	1:A:881:GLN:HG2	1.96	0.65
1:A:925:LEU:HD21	1:A:990:LEU:CB	2.25	0.65
1:B:516:LEU:HD12	1:B:557:LYS:HB2	1.78	0.65
1:B:601:LYS:HG2	1:B:613:ASN:HD21	1.61	0.65
1:B:822:GLU:O	1:B:826:LEU:HG	1.97	0.65
1:B:85:PHE:O	1:B:88:VAL:HG13	1.97	0.65
1:A:276:ARG:HG2	1:A:282:TYR:CZ	2.31	0.65
1:B:851:LEU:HD12	1:B:851:LEU:N	2.12	0.65
1:B:565:LYS:NZ	1:B:565:LYS:HB3	2.12	0.64
1:B:623:LYS:HZ3	1:B:625:ALA:HB3	1.61	0.64
1:A:775:ALA:O	1:A:779:VAL:HG23	1.97	0.64
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.79	0.64
1:A:948:SER:O	1:A:952:GLN:HG3	1.97	0.64
1:B:510:SER:O	1:B:514:ILE:HG13	1.96	0.64
1:B:914:THR:HG22	1:B:914:THR:O	1.97	0.64
1:B:2:ASN:ND2	1:B:4:ILE:HB	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:O	1:A:554:LYS:HG3	1.97	0.64
1:A:852:THR:CG2	1:A:855:GLU:H	2.10	0.64
1:B:709:ALA:HB2	1:B:726:VAL:HA	1.80	0.64
1:B:958:TYR:O	1:B:961:VAL:HG23	1.98	0.64
1:A:706:TYR:CE1	1:A:707:LEU:HG	2.33	0.63
1:B:692:PHE:CE1	1:B:747:ARG:HG2	2.32	0.63
1:B:59:SER:HB2	1:B:72:VAL:O	1.98	0.63
1:B:504:ILE:HD11	1:B:690:LYS:NZ	2.13	0.63
1:A:543:LEU:CD2	1:A:581:ILE:HD11	2.29	0.63
1:A:793:ASP:C	1:A:795:GLY:H	2.06	0.63
1:B:628:ILE:HG23	1:B:632:ALA:HB3	1.79	0.63
1:A:291:GLU:H	1:A:291:GLU:CD	2.07	0.63
1:B:273:GLU:CD	1:B:273:GLU:H	2.06	0.63
1:A:622:LYS:HE3	1:A:622:LYS:HA	1.79	0.63
1:B:718:ASP:OD1	1:B:721:LYS:HG3	1.99	0.63
1:B:18:LYS:N	1:B:18:LYS:HD2	2.14	0.63
1:B:123:LEU:HD22	1:B:158:ILE:HG13	1.81	0.63
1:B:562:ARG:HH22	1:B:563:PHE:HE1	1.46	0.63
1:A:893:ARG:NH1	1:A:897:LYS:HE3	2.14	0.62
1:B:924:LYS:HA	1:B:927:ASN:ND2	2.14	0.62
1:A:497:GLU:HB2	1:A:499:ILE:HD13	1.81	0.62
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.80	0.62
1:B:991:LEU:O	1:B:995:GLU:HG3	2.00	0.62
1:A:597:GLU:O	1:A:601:LYS:HB2	1.99	0.62
1:B:351:ILE:HG23	1:B:422:VAL:HG13	1.82	0.62
1:A:601:LYS:HG2	1:A:613:ASN:HD21	1.65	0.62
1:B:280:ILE:H	1:B:280:ILE:HD12	1.64	0.62
1:B:718:ASP:CG	1:B:721:LYS:HG3	2.25	0.62
1:A:493:GLU:HG2	1:A:695:ARG:NH1	2.15	0.61
1:A:984:GLU:C	1:A:986:TYR:H	2.08	0.61
1:B:59:SER:HA	1:B:74:LYS:H	1.64	0.61
1:B:899:GLU:HG3	1:B:975:GLN:HE22	1.65	0.61
1:A:839:LEU:C	1:A:841:LYS:N	2.56	0.61
1:B:91:MET:CE	1:B:106:LEU:HD13	2.30	0.61
1:B:715:ASP:O	1:B:716:ALA:HB2	2.00	0.61
1:B:534:VAL:HG22	1:B:534:VAL:O	2.00	0.61
1:A:538:ALA:HB1	1:A:542:THR:HG21	1.81	0.61
1:B:808:HIS:NE2	1:B:812:LYS:HE3	2.16	0.61
1:B:840:ILE:CG2	1:B:842:ARG:HG2	2.30	0.61
1:A:431:LEU:HD22	1:A:617:ILE:HG12	1.82	0.61
1:A:772:LEU:HD11	1:A:845:PHE:HZ	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:ASN:HD22	1:B:972:PHE:HE1	1.49	0.61
1:A:68:GLN:NE2	1:A:68:GLN:N	2.49	0.61
1:A:233:ASN:HD22	1:A:233:ASN:C	2.09	0.61
1:B:477:LYS:HB3	1:B:642:MET:HE2	1.82	0.60
1:B:928:LEU:HD13	1:B:928:LEU:O	2.01	0.60
1:B:961:VAL:HB	1:B:962:PRO:HD3	1.82	0.60
1:A:158:ILE:HG23	1:A:175:LEU:HD21	1.83	0.60
1:A:594:GLN:O	1:A:598:LEU:HG	2.02	0.60
1:B:6:ASP:O	1:B:8:THR:N	2.34	0.60
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.66	0.60
1:B:99:GLU:N	1:B:100:PRO:HD2	2.15	0.60
1:A:274:THR:O	1:A:274:THR:HG22	2.00	0.60
1:A:528:LEU:HD12	1:A:547:LEU:HD23	1.83	0.60
1:B:830:TYR:O	1:B:834:GLN:HG2	2.01	0.60
1:B:744:ILE:HD12	1:B:746:PHE:CZ	2.37	0.60
1:A:606:ASN:O	1:A:609:THR:HG22	2.01	0.60
1:B:789:LEU:O	1:B:870:HIS:HD2	1.85	0.59
1:A:459:GLU:OE1	1:A:471:ILE:HD12	2.02	0.59
1:A:697:ILE:HD11	1:A:700:ASP:OD1	2.02	0.59
1:B:217:GLN:O	1:B:220:PRO:HD2	2.02	0.59
1:A:623:LYS:NZ	1:A:625:ALA:HB3	2.17	0.59
1:B:369:LEU:CD2	1:B:375:LEU:HD12	2.33	0.59
1:A:496:LYS:O	1:A:741:ILE:HD12	2.03	0.59
1:B:775:ALA:HB3	1:B:851:LEU:HD23	1.83	0.59
1:B:846:VAL:HG13	1:B:846:VAL:O	2.02	0.59
1:A:40:ASP:C	1:A:42:ASP:H	2.11	0.59
1:B:98:ASN:O	1:B:102:VAL:HG23	2.03	0.59
1:A:566:THR:HB	1:A:580:GLU:OE1	2.03	0.59
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.33	0.59
1:A:487:PHE:CZ	1:A:506:PHE:HA	2.37	0.59
1:A:516:LEU:O	1:A:525:ILE:HG13	2.03	0.59
1:B:593:GLN:HB2	1:B:596:LEU:HD12	1.84	0.59
1:A:505:ASP:O	1:A:506:PHE:HB2	2.04	0.58
1:B:879:LYS:O	1:B:883:LYS:HB2	2.02	0.58
1:B:497:GLU:CD	1:B:742:THR:HG22	2.28	0.58
1:B:744:ILE:C	1:B:744:ILE:HD13	2.28	0.58
1:B:139:MET:HE2	1:B:142:ILE:HD12	1.85	0.58
1:B:73:LYS:HB2	1:B:73:LYS:NZ	2.19	0.58
1:A:994:LEU:HA	1:A:997:LEU:HB2	1.85	0.58
1:B:56:THR:C	1:B:58:ASP:H	2.11	0.58
1:A:913:GLU:HG3	1:A:920:ALA:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:928:LEU:HD13	2.04	0.58
1:A:507:GLY:O	1:A:508:LEU:HD13	2.04	0.58
1:B:68:GLN:HE22	1:B:70:ARG:HH21	1.52	0.58
1:B:45:ASP:HB3	1:B:673:LEU:HD12	1.85	0.57
1:B:459:GLU:HG3	1:B:471:ILE:HG21	1.85	0.57
1:A:2:ASN:N	1:A:3:PRO:HD3	2.19	0.57
1:A:879:LYS:O	1:A:883:LYS:HG3	2.04	0.57
1:B:213:GLN:HA	1:B:213:GLN:NE2	2.19	0.57
1:A:555:ASN:HD22	1:A:557:LYS:N	2.02	0.57
1:A:997:LEU:C	1:A:1001:GLU:HB2	2.29	0.57
1:B:543:LEU:CD2	1:B:581:ILE:HD11	2.29	0.57
1:B:620:ARG:O	1:B:621:ALA:HB2	2.05	0.57
1:A:217:GLN:C	1:A:220:PRO:HD2	2.29	0.57
1:B:562:ARG:HB3	1:B:562:ARG:HH11	1.70	0.57
1:B:819:LYS:O	1:B:823:VAL:HG23	2.03	0.57
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.20	0.57
1:B:73:LYS:HG3	1:B:75:ASP:H	1.69	0.57
1:A:529:LEU:O	1:A:529:LEU:HD23	2.04	0.57
1:A:924:LYS:C	1:A:926:LYS:H	2.13	0.57
1:B:270:PHE:HA	1:B:309:GLN:NE2	2.19	0.57
1:A:500:ASN:C	1:A:500:ASN:HD22	2.13	0.57
1:B:498:LYS:HB2	1:B:741:ILE:HD11	1.85	0.57
1:B:943:ASN:ND2	1:B:968:LYS:HE2	2.20	0.56
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.40	0.56
1:A:213:GLN:HA	1:A:213:GLN:HE21	1.70	0.56
1:A:497:GLU:CB	1:A:499:ILE:HD13	2.36	0.56
1:A:555:ASN:HD22	1:A:555:ASN:C	2.14	0.56
1:A:922:GLN:C	1:A:924:LYS:H	2.13	0.56
1:B:223:GLU:HG3	4:B:2206:HOH:O	2.04	0.56
1:A:410:ASN:HD22	1:A:411:VAL:H	1.52	0.56
1:A:507:GLY:O	1:A:508:LEU:O	2.23	0.56
1:B:878:LEU:HG	1:B:882:LYS:NZ	2.20	0.56
1:B:994:LEU:HD23	1:B:995:GLU:N	2.20	0.56
1:A:404:LEU:HD23	1:A:404:LEU:H	1.69	0.56
1:A:410:ASN:ND2	1:A:411:VAL:H	2.03	0.56
1:B:68:GLN:O	1:B:70:ARG:HG3	2.05	0.56
1:B:123:LEU:HD22	1:B:158:ILE:CG1	2.36	0.56
1:B:223:GLU:HG2	1:B:227:ASN:CG	2.30	0.56
1:B:994:LEU:HD23	1:B:994:LEU:C	2.30	0.56
1:B:905:LYS:CG	1:B:931:PHE:HE1	2.19	0.56
1:A:455:ILE:CD1	1:A:456:SER:H	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:HG3	1:A:521:GLN:N	2.21	0.55
1:A:793:ASP:CG	1:A:794:PHE:H	2.12	0.55
1:A:990:LEU:HD23	1:A:993:GLU:OE2	2.06	0.55
1:B:280:ILE:HD12	1:B:280:ILE:N	2.21	0.55
1:A:7:ARG:CD	1:A:21:ASP:HB3	2.35	0.55
1:B:562:ARG:NH1	1:B:562:ARG:CB	2.69	0.55
1:A:891:TYR:CE2	1:A:964:LEU:HD22	2.41	0.55
1:A:4:ILE:HD12	1:A:146:ARG:NH1	2.22	0.55
1:A:240:GLY:HA2	1:A:455:ILE:HD13	1.87	0.55
1:A:531:GLU:O	1:A:534:VAL:HG12	2.05	0.55
1:B:449:PHE:C	1:B:449:PHE:CD2	2.85	0.55
1:B:713:PRO:HG2	1:B:715:ASP:O	2.06	0.55
1:A:385:ASN:OD1	1:A:387:SER:HB2	2.07	0.55
1:A:130:LYS:HD2	1:B:302:GLU:HG3	1.89	0.55
1:A:421:LEU:O	1:A:425:LEU:HB2	2.08	0.54
1:A:431:LEU:HD23	1:A:431:LEU:O	2.07	0.54
1:B:402:ARG:HD3	1:B:402:ARG:N	2.22	0.54
1:B:496:LYS:O	1:B:497:GLU:HB3	2.07	0.54
1:B:669:ASP:OD2	1:B:670:LYS:N	2.40	0.54
1:A:280:ILE:HD12	1:A:281:PHE:H	1.72	0.54
1:A:508:LEU:O	1:A:508:LEU:HD22	2.07	0.54
1:A:816:LYS:HB3	1:A:817:PRO:HD3	1.89	0.54
1:B:980:LYS:O	1:B:983:ALA:HB3	2.08	0.54
1:A:811:TYR:O	1:A:811:TYR:CG	2.60	0.54
1:B:59:SER:HA	1:B:74:LYS:CB	2.37	0.54
1:A:213:GLN:HG3	1:A:333:ILE:HG21	1.90	0.54
1:A:1006:HIS:O	1:A:1010:HIS:HB2	2.08	0.54
1:B:35:ILE:O	1:B:49:CYS:HA	2.07	0.54
1:B:37:TYR:HE1	1:B:39:PRO:HA	1.72	0.54
1:B:60:PHE:CE1	1:B:74:LYS:HE2	2.43	0.54
1:B:305:ASN:ND2	1:B:356:ASN:HA	2.23	0.54
1:B:785:LYS:O	1:B:788:SER:HB3	2.08	0.54
1:A:379:SER:HB3	1:A:384:VAL:O	2.07	0.54
1:A:566:THR:O	1:A:581:ILE:HG22	2.07	0.54
1:A:916:ASP:O	1:A:917:SER:HB3	2.08	0.54
1:B:59:SER:HA	1:B:74:LYS:HB2	1.89	0.54
1:B:223:GLU:HG2	1:B:227:ASN:ND2	2.23	0.54
1:B:327:THR:O	1:B:331:MET:HG3	2.08	0.54
1:A:289:THR:O	1:A:293:LYS:HG3	2.08	0.53
1:B:499:ILE:HD11	1:B:740:GLY:CA	2.36	0.53
1:B:943:ASN:HD21	1:B:968:LYS:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:TYR:CE2	1:B:714:ARG:HG3	2.43	0.53
1:B:213:GLN:HA	1:B:213:GLN:HE21	1.72	0.53
1:B:398:ILE:HG22	1:B:405:VAL:O	2.09	0.53
1:A:515:ASP:C	1:A:517:ILE:N	2.66	0.53
1:A:903:THR:O	1:A:907:VAL:HG23	2.09	0.53
1:A:931:PHE:C	1:A:933:GLY:H	2.16	0.53
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.73	0.53
1:B:744:ILE:HD13	1:B:745:PHE:N	2.23	0.53
1:A:893:ARG:HH12	1:A:897:LYS:HE3	1.74	0.53
1:A:410:ASN:ND2	1:A:411:VAL:N	2.57	0.53
1:B:357:ILE:HD11	1:B:375:LEU:HA	1.89	0.53
1:B:109:ARG:O	1:B:114:LEU:HB2	2.09	0.53
1:A:217:GLN:O	1:A:220:PRO:HD2	2.09	0.53
1:A:354:LEU:O	1:A:418:ARG:NH1	2.41	0.53
1:A:592:LEU:HD23	1:A:597:GLU:OE2	2.09	0.53
1:A:793:ASP:O	1:A:795:GLY:N	2.42	0.53
1:A:798:ILE:N	1:A:798:ILE:HD12	2.24	0.53
1:B:33:ARG:O	1:B:52:ILE:HG12	2.09	0.53
1:B:210:VAL:O	1:B:214:GLN:HG3	2.08	0.53
1:B:558:TYR:CD2	1:B:559:GLU:N	2.77	0.52
1:A:744:ILE:HD13	1:A:745:PHE:N	2.24	0.52
1:A:797:SER:OG	1:A:798:ILE:N	2.42	0.52
1:A:520:ARG:HA	1:A:520:ARG:NH1	2.23	0.52
1:A:622:LYS:CE	1:A:624:GLY:H	2.17	0.52
1:A:327:THR:HG22	1:A:331:MET:CE	2.40	0.52
1:A:544:ILE:HG12	1:A:548:HIS:NE2	2.25	0.52
1:A:796:ASP:O	1:A:796:ASP:OD2	2.28	0.52
1:A:926:LYS:O	1:A:926:LYS:HD3	2.09	0.52
1:B:296:LEU:HB2	1:B:298:LEU:HG	1.90	0.52
1:B:626:ASN:CG	1:B:627:PHE:H	2.18	0.52
1:B:872:GLU:HA	1:B:872:GLU:OE1	2.10	0.52
1:B:696:ILE:O	1:B:743:LYS:HB2	2.10	0.52
1:B:798:ILE:N	1:B:798:ILE:HD12	2.24	0.52
1:A:793:ASP:C	1:A:795:GLY:N	2.67	0.52
1:A:917:SER:O	1:A:997:LEU:HD13	2.09	0.52
1:A:59:SER:N	1:A:74:LYS:HG3	2.25	0.52
1:A:280:ILE:HD12	1:A:281:PHE:N	2.24	0.52
1:B:6:ASP:C	1:B:8:THR:H	2.17	0.52
1:B:201:GLY:O	1:B:203:ASN:N	2.43	0.52
1:B:899:GLU:HA	1:B:971:PHE:HZ	1.75	0.52
1:B:918:ILE:CG1	1:B:997:LEU:HD22	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.24	0.52
1:A:507:GLY:C	1:A:508:LEU:HD13	2.35	0.52
1:B:45:ASP:CG	1:B:677:ARG:HH22	2.17	0.51
1:B:531:GLU:O	1:B:534:VAL:HG12	2.09	0.51
1:A:987:LYS:O	1:A:987:LYS:HD3	2.09	0.51
1:B:115:ILE:HG21	1:B:128:PRO:HB3	1.91	0.51
1:B:909:LEU:HD22	1:B:983:ALA:HA	1.92	0.51
1:B:565:LYS:HB3	1:B:565:LYS:HZ2	1.74	0.51
1:B:375:LEU:O	1:B:375:LEU:HD23	2.10	0.51
1:B:562:ARG:HB2	1:B:562:ARG:CZ	2.40	0.51
1:B:573:TYR:OH	1:B:683:GLU:OE2	2.29	0.51
1:A:115:ILE:HD13	1:A:132:ILE:HD11	1.92	0.51
1:A:357:ILE:HG23	1:A:369:LEU:HD11	1.92	0.51
1:A:404:LEU:H	1:A:404:LEU:CD2	2.24	0.51
1:A:589:LYS:HD2	1:A:591:PRO:HB3	1.93	0.51
1:A:892:ASN:HB3	1:A:896:LYS:HZ2	1.75	0.51
1:A:896:LYS:O	1:A:900:ASN:ND2	2.44	0.51
1:B:95:SER:HB3	1:B:752:ALA:HB2	1.93	0.51
1:B:497:GLU:OE2	1:B:742:THR:HG22	2.10	0.51
1:A:666:LYS:HE2	1:A:666:LYS:CA	2.38	0.51
1:A:736:GLN:HB3	1:A:750:GLN:HG2	1.92	0.51
1:A:162:ALA:O	1:A:173:GLN:HG3	2.10	0.51
1:A:372:LYS:HD2	1:A:372:LYS:N	2.25	0.51
1:B:244:GLU:O	1:B:256:ALA:HA	2.11	0.51
1:B:918:ILE:CD1	1:B:998:GLN:HA	2.41	0.51
1:B:270:PHE:HA	1:B:309:GLN:HE22	1.76	0.51
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.93	0.51
1:A:655:CYS:C	1:A:656:ILE:HD12	2.36	0.51
1:A:850:GLY:O	1:A:851:LEU:HD13	2.11	0.51
1:B:477:LYS:HD3	1:B:514:ILE:HD13	1.92	0.51
1:A:622:LYS:HE3	1:A:623:LYS:H	1.76	0.50
1:B:99:GLU:H	1:B:100:PRO:HD2	1.74	0.50
1:B:840:ILE:HD13	1:B:840:ILE:O	2.11	0.50
1:A:40:ASP:C	1:A:42:ASP:N	2.70	0.50
1:B:909:LEU:HD13	1:B:983:ALA:HA	1.93	0.50
1:B:993:GLU:O	1:B:997:LEU:HB2	2.10	0.50
1:A:901:TRP:NE1	1:A:935:CYS:SG	2.84	0.50
1:A:911:SER:O	1:A:911:SER:OG	2.25	0.50
1:A:61:THR:HG23	1:A:71:GLN:HG2	1.93	0.50
1:A:500:ASN:C	1:A:500:ASN:ND2	2.70	0.50
1:B:744:ILE:HD12	1:B:746:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:ND2	1:A:149:ASN:C	2.69	0.50
1:B:520:ARG:HG2	1:B:520:ARG:HH11	1.77	0.50
1:A:143:PHE:HA	1:A:146:ARG:HG3	1.94	0.50
1:A:204:GLN:O	1:A:205:ALA:HB3	2.12	0.50
1:A:398:ILE:HD13	1:A:407:GLN:HB2	1.94	0.49
1:A:510:SER:O	1:A:514:ILE:HG13	2.12	0.49
1:A:817:PRO:HB2	1:A:818:PRO:CD	2.37	0.49
1:A:918:ILE:HG22	1:A:918:ILE:O	2.11	0.49
1:A:499:ILE:HD11	1:A:740:GLY:CA	2.43	0.49
1:A:520:ARG:HG3	1:A:521:GLN:CG	2.39	0.49
1:A:852:THR:HG22	1:A:855:GLU:H	1.75	0.49
1:A:68:GLN:HE21	1:A:68:GLN:N	2.03	0.49
1:A:925:LEU:CD1	1:A:990:LEU:HD13	2.41	0.49
1:B:135:TYR:CD1	1:B:191:LYS:HD2	2.47	0.49
1:B:496:LYS:O	1:B:497:GLU:CB	2.61	0.49
1:B:735:GLU:O	1:B:747:ARG:HD2	2.12	0.49
1:B:794:PHE:O	1:B:800:SER:OG	2.26	0.49
1:A:149:ASN:C	1:A:149:ASN:HD22	2.20	0.49
1:A:588:ASN:HA	1:A:630:VAL:HB	1.93	0.49
1:A:962:PRO:HB2	1:A:963:GLU:OE2	2.13	0.49
1:B:688:THR:O	1:B:693:PRO:HG3	2.12	0.49
1:A:7:ARG:NE	1:A:21:ASP:HB3	2.27	0.49
1:A:449:PHE:C	1:A:449:PHE:CD2	2.90	0.49
1:A:515:ASP:C	1:A:517:ILE:H	2.20	0.49
1:B:696:ILE:HG22	1:B:697:ILE:O	2.12	0.49
1:B:1007:HIS:ND1	1:B:1007:HIS:C	2.69	0.49
1:A:697:ILE:HG12	1:A:697:ILE:O	2.13	0.49
1:B:568:PHE:CD1	1:B:568:PHE:C	2.91	0.49
1:B:620:ARG:HG3	1:B:633:GLN:OE1	2.13	0.49
1:A:589:LYS:HD3	1:A:589:LYS:C	2.36	0.49
1:B:136:THR:O	1:B:140:VAL:HG23	2.12	0.49
1:A:410:ASN:HD21	1:A:412:GLU:HG3	1.78	0.49
1:A:692:PHE:CE1	1:A:747:ARG:HG3	2.47	0.49
1:B:273:GLU:O	1:B:274:THR:CB	2.61	0.49
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.78	0.49
1:A:622:LYS:HE3	1:A:623:LYS:N	2.28	0.49
1:A:124:VAL:HG13	1:A:656:ILE:HD13	1.94	0.48
1:A:398:ILE:N	1:A:398:ILE:HD12	2.28	0.48
1:A:622:LYS:HE2	1:A:624:GLY:N	2.22	0.48
1:A:811:TYR:HD1	1:A:815:GLU:HB2	1.78	0.48
1:B:139:MET:CE	1:B:142:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:GLU:HG3	1:A:994:LEU:HD22	1.94	0.48
1:B:2:ASN:HD21	1:B:4:ILE:HB	1.76	0.48
1:B:47:TYR:CD2	1:B:100:PRO:HB3	2.49	0.48
1:B:505:ASP:O	1:B:507:GLY:N	2.43	0.48
1:B:656:ILE:HD12	1:B:656:ILE:N	2.29	0.48
1:A:354:LEU:HD11	1:A:382:PHE:HE1	1.78	0.48
1:B:532:GLN:HG2	1:B:543:LEU:HB2	1.94	0.48
1:B:223:GLU:O	1:B:227:ASN:HB2	2.13	0.48
1:B:840:ILE:O	1:B:841:LYS:HB2	2.14	0.48
1:B:1005:HIS:O	1:B:1005:HIS:ND1	2.46	0.48
1:A:697:ILE:O	1:A:698:TYR:C	2.57	0.48
1:A:761:ARG:O	1:A:764:SER:HB3	2.13	0.48
1:A:852:THR:HG23	1:A:854:ASN:H	1.78	0.48
1:A:981:SER:O	1:A:984:GLU:HB2	2.14	0.48
1:B:562:ARG:NH1	1:B:562:ARG:HB2	2.27	0.48
1:A:468:GLN:N	1:A:468:GLN:OE1	2.47	0.48
1:A:894:ILE:O	1:A:897:LYS:HB2	2.14	0.48
1:A:919:THR:HA	1:A:923:ALA:HB3	1.96	0.48
1:B:95:SER:CB	1:B:752:ALA:HB2	2.43	0.48
1:B:505:ASP:O	1:B:506:PHE:CD1	2.67	0.48
1:A:431:LEU:HD23	1:A:431:LEU:C	2.38	0.48
1:A:520:ARG:NH1	1:A:520:ARG:HB2	2.29	0.48
1:A:985:THR:HG22	1:A:985:THR:O	2.14	0.48
1:B:140:VAL:HG13	1:B:195:TYR:CD1	2.49	0.48
1:B:742:THR:CG2	1:B:743:LYS:HE3	2.44	0.48
1:A:626:ASN:O	1:A:627:PHE:O	2.31	0.48
1:B:546:LYS:HE2	1:B:550:HIS:CE1	2.48	0.48
1:A:223:GLU:O	1:A:227:ASN:HB2	2.14	0.48
1:A:943:ASN:HD21	1:A:968:LYS:NZ	2.12	0.48
1:B:249:ASN:OD1	1:B:250:ALA:N	2.47	0.48
1:A:921:VAL:CG1	1:A:994:LEU:HD21	2.43	0.47
1:B:243:ILE:HD13	1:B:243:ILE:N	2.27	0.47
1:B:852:THR:CG2	1:B:855:GLU:HB2	2.44	0.47
1:A:176:LEU:N	1:A:176:LEU:HD12	2.30	0.47
1:A:507:GLY:O	1:A:508:LEU:C	2.56	0.47
1:A:943:ASN:O	1:A:947:LEU:HG	2.14	0.47
1:B:361:LYS:HA	1:B:361:LYS:CE	2.44	0.47
1:A:846:VAL:HG12	1:A:846:VAL:O	2.14	0.47
1:B:296:LEU:CD2	1:B:346:LYS:HG2	2.45	0.47
1:B:472:ASN:O	1:B:476:GLU:HG2	2.15	0.47
1:B:34:TYR:HA	1:B:50:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LYS:HE2	1:B:703:LYS:C	2.40	0.47
1:A:375:LEU:HD11	1:A:390:GLU:HB2	1.96	0.47
1:A:990:LEU:O	1:A:994:LEU:HD23	2.13	0.47
1:A:1000:ILE:HG22	1:A:1000:ILE:O	2.14	0.47
1:A:270:PHE:C	1:A:271:GLN:NE2	2.73	0.47
1:A:520:ARG:HH11	1:A:520:ARG:CA	2.26	0.47
1:B:496:LYS:C	1:B:498:LYS:N	2.68	0.47
1:B:620:ARG:HG2	1:B:620:ARG:HH11	1.80	0.47
1:B:833:LEU:O	1:B:833:LEU:HD12	2.14	0.47
1:A:233:ASN:ND2	1:A:233:ASN:C	2.73	0.47
1:B:207:GLY:O	1:B:210:VAL:HB	2.14	0.47
1:B:733:ASP:HA	1:B:734:PRO:HD2	1.83	0.47
1:B:850:GLY:N	1:B:855:GLU:OE1	2.44	0.47
1:A:482:PHE:CD1	1:A:482:PHE:C	2.93	0.47
1:B:18:LYS:HD3	1:B:112:GLN:OE1	2.14	0.47
1:B:812:LYS:C	1:B:813:LYS:HD2	2.39	0.47
1:A:727:LEU:HD12	1:A:732:ILE:HD12	1.95	0.47
1:B:516:LEU:HD12	1:B:557:LYS:CB	2.45	0.47
1:B:816:LYS:HB3	1:B:817:PRO:HD3	1.96	0.47
1:A:628:ILE:HG13	1:A:632:ALA:CB	2.42	0.46
1:B:733:ASP:C	1:B:735:GLU:H	2.24	0.46
1:B:785:LYS:HE2	1:B:811:TYR:CE1	2.50	0.46
1:A:6:ASP:O	1:A:8:THR:N	2.48	0.46
1:A:956:LEU:O	1:A:957:ASN:C	2.57	0.46
1:B:375:LEU:HD23	1:B:375:LEU:C	2.40	0.46
1:B:398:ILE:HG12	1:B:399:LEU:N	2.30	0.46
1:A:369:LEU:CD2	1:A:375:LEU:HD12	2.45	0.46
1:B:241:LYS:HA	1:B:259:GLN:O	2.16	0.46
1:B:851:LEU:C	1:B:852:THR:HG22	2.41	0.46
1:B:924:LYS:HA	1:B:927:ASN:HD22	1.81	0.46
1:A:87:GLY:H	1:A:105:ASN:ND2	2.12	0.46
1:A:369:LEU:C	1:A:371:ASP:H	2.23	0.46
1:A:372:LYS:O	1:A:373:THR:C	2.57	0.46
1:A:695:ARG:HD2	1:A:695:ARG:N	2.31	0.46
1:A:945:ASP:O	1:A:949:ILE:HG13	2.14	0.46
1:B:698:TYR:CE2	1:B:744:ILE:HB	2.51	0.46
1:B:894:ILE:CG2	1:B:946:LEU:HD21	2.45	0.46
1:A:892:ASN:O	1:A:896:LYS:HG3	2.16	0.46
1:B:4:ILE:HD11	1:B:151:VAL:HG12	1.98	0.46
1:A:63:LYS:O	1:A:64:THR:C	2.59	0.46
1:A:499:ILE:HD11	1:A:740:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LEU:C	1:B:375:LEU:CD2	2.89	0.46
1:B:395:GLU:HG2	1:B:407:GLN:O	2.16	0.46
1:B:483:ASN:HB3	1:B:506:PHE:HE1	1.81	0.46
1:A:798:ILE:N	1:A:798:ILE:CD1	2.79	0.46
1:B:98:ASN:N	1:B:98:ASN:ND2	2.61	0.46
1:B:878:LEU:O	1:B:882:LYS:HG2	2.16	0.46
1:B:979:VAL:HG23	1:B:980:LYS:N	2.31	0.46
1:A:7:ARG:NH1	1:A:7:ARG:HB2	2.31	0.46
1:A:851:LEU:N	1:A:851:LEU:HD22	2.31	0.46
1:A:992:ALA:HA	1:A:995:GLU:HG3	1.98	0.46
1:B:233:ASN:HD21	3:B:2100:ADP:H5'2	1.80	0.46
1:B:562:ARG:HH11	1:B:562:ARG:CB	2.28	0.46
1:B:755:GLU:O	1:B:759:GLU:HG3	2.16	0.46
1:A:85:PHE:O	1:A:88:VAL:HG13	2.16	0.45
1:A:334:VAL:HG12	1:A:334:VAL:O	2.15	0.45
1:A:811:TYR:O	1:A:812:LYS:HG3	2.15	0.45
1:A:852:THR:HG23	1:A:855:GLU:H	1.82	0.45
1:A:976:TRP:O	1:A:980:LYS:HB2	2.16	0.45
1:B:32:LYS:HD3	1:B:51:GLU:CD	2.41	0.45
1:B:147:ARG:HD2	1:B:150:GLU:OE1	2.16	0.45
1:B:205:ALA:HB3	1:B:208:SER:OG	2.16	0.45
1:B:409:LEU:N	1:B:409:LEU:HD23	2.32	0.45
1:B:878:LEU:HG	1:B:882:LYS:HZ2	1.81	0.45
1:A:421:LEU:HD21	1:A:600:PHE:CE1	2.52	0.45
1:A:497:GLU:HB3	1:A:499:ILE:CD1	2.46	0.45
1:B:302:GLU:CD	1:B:302:GLU:H	2.24	0.45
1:B:785:LYS:HE2	1:B:811:TYR:CD1	2.51	0.45
1:A:520:ARG:HB2	1:A:520:ARG:CZ	2.46	0.45
1:A:589:LYS:O	1:A:590:ASP:C	2.60	0.45
1:B:692:PHE:CD1	1:B:747:ARG:HG2	2.51	0.45
1:B:852:THR:HG23	1:B:855:GLU:HB2	1.97	0.45
1:B:40:ASP:C	1:B:42:ASP:H	2.25	0.45
1:B:294:LYS:O	1:B:294:LYS:HG3	2.15	0.45
1:B:397:ARG:HA	1:B:406:ALA:HA	1.99	0.45
1:B:490:GLU:OE1	1:B:490:GLU:HA	2.16	0.45
1:B:217:GLN:C	1:B:220:PRO:HD2	2.42	0.45
1:B:362:GLY:HA2	1:B:368:VAL:HG22	1.98	0.45
1:B:715:ASP:O	1:B:716:ALA:CB	2.64	0.45
1:A:752:ALA:O	1:A:756:GLU:HG3	2.16	0.45
1:A:901:TRP:C	1:A:903:THR:H	2.24	0.45
1:B:99:GLU:N	1:B:100:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:928:LEU:HD23	1:B:986:TYR:HD1	1.82	0.45
1:B:979:VAL:O	1:B:983:ALA:N	2.49	0.45
1:B:366:GLY:HA3	1:B:408:HIS:CE1	2.51	0.45
1:B:733:ASP:O	1:B:735:GLU:N	2.50	0.45
1:B:548:HIS:O	1:B:552:SER:HB3	2.17	0.44
1:B:968:LYS:NZ	1:B:968:LYS:HB3	2.32	0.44
1:B:331:MET:HE1	1:B:344:ILE:HD12	2.00	0.44
1:A:539:THR:N	1:A:542:THR:HG22	2.32	0.44
1:A:562:ARG:HD2	1:A:563:PHE:CE1	2.52	0.44
1:B:638:LEU:HD12	1:B:638:LEU:O	2.17	0.44
1:A:146:ARG:HE	1:A:146:ARG:HB3	1.53	0.44
1:A:230:THR:HB	1:A:275:GLU:OE2	2.17	0.44
1:A:383:GLY:O	1:A:603:SER:HA	2.18	0.44
1:A:548:HIS:ND1	1:A:560:GLU:HG3	2.33	0.44
1:A:785:LYS:HB2	1:A:785:LYS:NZ	2.32	0.44
1:A:922:GLN:HB2	1:A:994:LEU:CD1	2.46	0.44
1:B:369:LEU:HD23	1:B:375:LEU:HD12	1.99	0.44
1:B:592:LEU:O	1:B:593:GLN:C	2.59	0.44
1:B:851:LEU:N	1:B:851:LEU:CD1	2.77	0.44
1:B:918:ILE:HD11	1:B:998:GLN:CA	2.43	0.44
1:A:395:GLU:HG2	1:A:408:HIS:ND1	2.32	0.44
1:B:798:ILE:O	1:B:799:GLU:C	2.58	0.44
1:A:397:ARG:HA	1:A:406:ALA:HA	2.00	0.44
1:A:931:PHE:C	1:A:933:GLY:N	2.75	0.44
1:B:934:GLU:HA	1:B:937:SER:OG	2.17	0.44
1:A:229:LYS:HG3	1:A:234:ASN:HA	2.00	0.44
1:A:243:ILE:HD12	1:A:258:ILE:HG12	1.99	0.44
1:A:738:ARG:HA	1:A:738:ARG:HD3	1.77	0.44
1:B:696:ILE:HD12	1:B:696:ILE:N	2.32	0.44
1:B:37:TYR:CD1	1:B:37:TYR:C	2.95	0.44
1:B:661:LYS:HE3	1:B:663:LEU:HD12	1.99	0.44
1:B:1004:HIS:O	1:B:1004:HIS:CD2	2.71	0.44
1:A:40:ASP:O	1:A:42:ASP:N	2.51	0.44
1:A:729:HIS:C	1:A:731:ASN:H	2.26	0.44
1:A:768:LYS:O	1:A:772:LEU:HD13	2.17	0.44
1:B:170:ARG:HG3	1:B:448:TYR:OH	2.18	0.44
1:A:840:ILE:HG22	1:A:840:ILE:O	2.17	0.43
1:A:963:GLU:CD	1:A:963:GLU:H	2.25	0.43
1:B:112:GLN:O	1:B:113:ASP:HB2	2.18	0.43
1:B:736:GLN:HA	1:B:747:ARG:HG3	2.00	0.43
1:B:761:ARG:CZ	1:B:842:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:VAL:HG11	1:B:994:LEU:HB2	2.01	0.43
1:B:91:MET:HE3	1:B:106:LEU:HD13	1.99	0.43
1:B:248:ASN:OD1	1:B:248:ASN:C	2.61	0.43
1:B:398:ILE:HG12	1:B:399:LEU:H	1.83	0.43
1:B:898:LEU:HB3	1:B:971:PHE:CE2	2.53	0.43
1:A:703:LYS:HG3	1:A:714:ARG:NH2	2.33	0.43
1:A:713:PRO:HD2	1:A:716:ALA:HB2	2.00	0.43
1:A:148:ARG:HG3	1:A:148:ARG:NH1	2.31	0.43
1:A:622:LYS:HE3	1:A:622:LYS:CA	2.47	0.43
1:A:834:GLN:OE1	1:A:834:GLN:HA	2.19	0.43
1:B:68:GLN:HE22	1:B:70:ARG:NH2	2.16	0.43
1:B:229:LYS:HD3	1:B:229:LYS:C	2.43	0.43
1:B:620:ARG:O	1:B:621:ALA:CB	2.66	0.43
1:B:43:GLU:OE1	1:B:670:LYS:HD2	2.19	0.43
1:B:905:LYS:HB3	1:B:931:PHE:HE1	1.84	0.43
1:A:95:SER:HA	1:A:694:ASN:HD21	1.83	0.43
1:A:158:ILE:CG2	1:A:175:LEU:HD21	2.49	0.43
1:A:418:ARG:C	1:A:418:ARG:HD2	2.44	0.43
1:A:732:ILE:HD11	1:A:754:ILE:HG12	1.99	0.43
1:A:937:SER:C	1:A:939:GLU:H	2.27	0.43
1:A:961:VAL:N	1:A:962:PRO:CD	2.81	0.43
1:B:626:ASN:CG	1:B:627:PHE:N	2.76	0.43
1:A:116:TYR:HE2	1:A:188:ASN:HD21	1.66	0.43
1:A:327:THR:HG22	1:A:331:MET:HE2	2.00	0.43
1:A:539:THR:H	1:A:542:THR:HG22	1.83	0.43
1:A:982:SER:C	1:A:984:GLU:H	2.26	0.43
1:B:405:VAL:O	1:B:405:VAL:HG23	2.18	0.43
1:A:279:HIS:O	1:A:283:GLN:HG3	2.19	0.43
1:B:503:PHE:HE1	1:B:690:LYS:HB2	1.84	0.43
1:A:626:ASN:O	1:A:627:PHE:C	2.62	0.43
1:B:737:TYR:HB2	1:B:744:ILE:HD11	2.01	0.43
1:A:185:LYS:HB2	1:A:185:LYS:HE2	1.82	0.43
1:A:350:GLY:HA3	1:A:382:PHE:CE2	2.53	0.43
1:A:360:GLU:OE2	1:A:370:LYS:HD2	2.19	0.43
1:B:702:VAL:HG21	1:B:722:ALA:HB3	2.00	0.43
1:B:372:LYS:O	1:B:376:ASN:ND2	2.52	0.42
1:B:410:ASN:O	1:B:411:VAL:C	2.62	0.42
1:B:529:LEU:HD13	1:B:543:LEU:HD21	2.01	0.42
1:B:87:GLY:H	1:B:105:ASN:ND2	2.17	0.42
1:B:823:VAL:HG21	1:B:860:TRP:CE3	2.53	0.42
1:A:7:ARG:CB	1:A:7:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:TRP:CZ2	1:A:935:CYS:SG	3.13	0.42
1:A:970:THR:O	1:A:974:GLN:HB2	2.19	0.42
1:B:40:ASP:C	1:B:42:ASP:N	2.76	0.42
1:B:473:TYR:O	1:B:476:GLU:HB2	2.19	0.42
1:A:88:VAL:N	1:A:105:ASN:HD21	2.17	0.42
1:A:233:ASN:HB3	1:A:236:SER:HB2	2.01	0.42
1:A:351:ILE:CG2	1:A:422:VAL:HG13	2.46	0.42
1:A:570:VAL:HG22	1:A:579:TYR:HE2	1.83	0.42
1:A:918:ILE:HG23	1:A:922:GLN:NE2	2.29	0.42
1:A:924:LYS:HE3	1:A:924:LYS:HB3	1.94	0.42
1:A:412:GLU:OE2	1:A:413:LYS:HG3	2.20	0.42
1:A:893:ARG:HH11	1:A:893:ARG:HG2	1.83	0.42
1:A:1002:ASP:HA	1:A:1005:HIS:HB3	2.02	0.42
1:B:424:ALA:O	1:B:428:ARG:HG3	2.19	0.42
1:A:610:LYS:HD3	1:A:614:ASP:HB2	2.02	0.42
1:B:620:ARG:HG2	1:B:620:ARG:NH1	2.35	0.42
1:B:816:LYS:O	1:B:817:PRO:C	2.62	0.42
1:B:970:THR:O	1:B:971:PHE:C	2.63	0.42
1:B:102:VAL:HG21	1:B:685:ILE:HD13	2.02	0.42
1:B:340:GLU:O	1:B:343:SER:HB2	2.20	0.42
1:B:852:THR:O	1:B:853:PRO:C	2.61	0.42
1:B:866:ALA:O	1:B:870:HIS:HB2	2.20	0.42
1:B:1007:HIS:HA	1:B:1010:HIS:NE2	2.34	0.42
1:A:158:ILE:HD12	1:A:158:ILE:HA	1.94	0.42
1:A:838:ARG:C	1:A:839:LEU:O	2.61	0.42
1:B:557:LYS:HD3	1:B:557:LYS:HA	1.83	0.42
1:A:504:ILE:O	1:A:504:ILE:HG13	2.20	0.42
1:A:801:VAL:O	1:A:805:MET:HG3	2.19	0.42
1:B:642:MET:O	1:B:646:GLU:HG3	2.20	0.42
1:A:237:SER:HB2	4:A:1203:HOH:O	2.18	0.41
1:A:455:ILE:HD12	1:A:456:SER:N	2.25	0.41
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.02	0.41
1:A:676:LEU:HD23	1:A:679:ASN:HD21	1.85	0.41
1:A:879:LYS:HE2	1:A:879:LYS:HB3	1.94	0.41
1:A:924:LYS:C	1:A:926:LYS:N	2.78	0.41
1:B:984:GLU:O	1:B:987:LYS:N	2.53	0.41
1:A:623:LYS:HZ1	1:A:625:ALA:HB3	1.85	0.41
1:B:36:TRP:CZ3	1:B:49:CYS:HB3	2.56	0.41
1:B:362:GLY:C	1:B:364:GLY:N	2.77	0.41
1:B:470:CYS:HB3	1:B:634:TYR:CE1	2.55	0.41
1:B:785:LYS:HD2	1:B:785:LYS:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ASN:O	1:B:896:LYS:HG3	2.20	0.41
1:B:912:ASN:ND2	1:B:912:ASN:C	2.77	0.41
1:B:708:LEU:HD13	1:B:730:LEU:HD11	2.03	0.41
1:B:792:ARG:HA	1:B:794:PHE:CZ	2.55	0.41
1:B:962:PRO:O	1:B:966:GLU:HG3	2.21	0.41
1:A:546:LYS:NZ	1:A:546:LYS:HB2	2.34	0.41
1:B:505:ASP:C	1:B:507:GLY:H	2.29	0.41
1:B:852:THR:HG21	1:B:855:GLU:OE2	2.20	0.41
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.92	0.41
1:A:33:ARG:O	1:A:52:ILE:HG13	2.20	0.41
1:A:97:LEU:O	1:A:689:ARG:NH1	2.52	0.41
1:B:666:LYS:HE3	1:B:666:LYS:HB3	1.95	0.41
1:A:35:ILE:O	1:A:49:CYS:HA	2.21	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.81	0.41
1:A:435:LYS:C	1:A:435:LYS:CD	2.94	0.41
1:B:7:ARG:HD2	1:B:12:HIS:CE1	2.56	0.41
1:B:233:ASN:ND2	3:B:2100:ADP:H5'2	2.36	0.41
1:B:340:GLU:O	1:B:344:ILE:HG13	2.21	0.41
1:B:589:LYS:HB2	1:B:589:LYS:HE3	1.86	0.41
1:A:321:GLU:H	1:A:321:GLU:HG3	1.57	0.41
1:A:538:ALA:CB	1:A:542:THR:HG21	2.49	0.41
1:A:614:ASP:OD1	1:A:614:ASP:C	2.64	0.41
1:B:45:ASP:OD2	1:B:677:ARG:NH2	2.47	0.41
1:B:523:PRO:O	1:B:551:PHE:HZ	2.03	0.41
1:B:776:ASN:CG	1:B:851:LEU:HD21	2.46	0.41
1:B:928:LEU:CD2	1:B:986:TYR:HD1	2.35	0.41
1:A:435:LYS:C	1:A:435:LYS:HD3	2.46	0.40
1:A:852:THR:HG23	1:A:854:ASN:N	2.36	0.40
1:B:82:PRO:HD2	1:B:85:PHE:CD1	2.56	0.40
1:B:123:LEU:CD2	1:B:158:ILE:HG13	2.48	0.40
1:B:182:GLY:HA2	1:B:233:ASN:HD22	1.86	0.40
1:A:257:SER:HA	1:A:438:ASN:OD1	2.21	0.40
1:A:812:LYS:HG2	1:A:816:LYS:HD2	2.04	0.40
1:A:848:PRO:CB	1:A:851:LEU:HD23	2.36	0.40
1:B:65:VAL:HG12	1:B:65:VAL:O	2.20	0.40
1:B:446:LYS:O	1:B:446:LYS:HG3	2.20	0.40
1:B:851:LEU:O	1:B:852:THR:CB	2.70	0.40
1:A:565:LYS:HD3	1:A:565:LYS:HA	1.85	0.40
1:B:276:ARG:HB3	1:B:282:TYR:CE2	2.56	0.40
1:B:736:GLN:O	1:B:747:ARG:HG3	2.21	0.40
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.83	0.40
1:A:937:SER:C	1:A:939:GLU:N	2.80	0.40
1:B:52:ILE:HD12	1:B:60:PHE:CD2	2.56	0.40
1:B:772:LEU:HD11	1:B:845:PHE:HZ	1.86	0.40
1:B:992:ALA:HA	1:B:995:GLU:OE1	2.21	0.40
1:B:1004:HIS:C	1:B:1006:HIS:N	2.78	0.40
1:A:364:GLY:C	1:A:366:GLY:N	2.79	0.40
1:A:642:MET:O	1:A:646:GLU:HG3	2.22	0.40
1:A:643:ALA:O	1:A:647:THR:HG23	2.21	0.40
1:A:785:LYS:HG3	1:A:863:LEU:HD11	2.04	0.40
1:B:56:THR:C	1:B:58:ASP:N	2.76	0.40

There are no symmetry-related clashes.

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	1007/1010 (100%)	887 (88%)	88 (9%)	32 (3%)	3	11
1	B	1007/1010 (100%)	875 (87%)	104 (10%)	28 (3%)	4	14
All	All	2014/2020 (100%)	1762 (88%)	192 (10%)	60 (3%)	3	12

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	203	ASN
1	A	204	GLN
1	A	508	LEU
1	A	536	PRO
1	A	621	ALA
1	A	627	PHE

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Mol	Chain	Res	Type
1	A	812	LYS
1	A	840	ILE
1	A	917	SER
1	B	7	ARG
1	B	24	LEU
1	B	64	THR
1	B	203	ASN
1	B	206	ASN
1	B	506	PHE
1	B	621	ALA
1	B	716	ALA
1	B	852	THR
1	A	7	ARG
1	A	370	LYS
1	A	698	TYR
1	A	794	PHE
1	A	796	ASP
1	A	911	SER
1	B	26	LYS
1	B	27	LEU
1	B	202	ARG
1	B	973	ALA
1	A	6	ASP
1	A	67	GLY
1	A	145	GLY
1	B	19	GLN
1	B	67	GLY
1	B	204	GLN
1	B	734	PRO
1	B	917	SER
1	A	504	ILE
1	A	599	CYS
1	A	925	LEU
1	A	957	ASN
1	A	960	GLY
1	B	69	ASP
1	B	959	ASN
1	A	39	PRO
1	A	59	SER
1	A	625	ALA
1	A	839	LEU
1	A	923	ALA

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Mol	Chain	Res	Type
1	A	985	THR
1	B	6	ASP
1	B	731	ASN
1	B	83	ILE
1	B	264	GLU
1	B	274	THR
1	B	554	LYS
1	A	710	PRO
1	B	411	VAL
1	B	53	VAL
1	A	848	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	884/885 (100%)	816 (92%)	68 (8%)	12	36
1	B	884/885 (100%)	825 (93%)	59 (7%)	15	42
All	All	1768/1770 (100%)	1641 (93%)	127 (7%)	13	39

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	38	ASN
1	A	44	ARG
1	A	68	GLN
1	A	146	ARG
1	A	148	ARG
1	A	149	ASN
1	A	158	ILE
1	A	175	LEU
1	A	185	LYS
1	A	196	LEU
1	A	213	GLN

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	264	GLU
1	A	274	THR
1	A	276	ARG
1	A	280	ILE
1	A	291	GLU
1	A	329	GLN
1	A	352	LEU
1	A	403	ASP
1	A	425	LEU
1	A	445	ARG
1	A	468	GLN
1	A	495	LEU
1	A	508	LEU
1	A	516	LEU
1	A	520	ARG
1	A	531	GLU
1	A	536	PRO
1	A	546	LYS
1	A	555	ASN
1	A	559	GLU
1	A	562	ARG
1	A	566	THR
1	A	585	LEU
1	A	610	LYS
1	A	622	LYS
1	A	666	LYS
1	A	683	GLU
1	A	690	LYS
1	A	697	ILE
1	A	710	PRO
1	A	727	LEU
1	A	744	ILE
1	A	753	ARG
1	A	758	ARG
1	A	767	THR
1	A	780	GLN
1	A	785	LYS
1	A	790	GLU
1	A	791	SER
1	A	793	ASP
1	A	797	SER

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Mol	Chain	Res	Type
1	A	804	PHE
1	A	806	ASN
1	A	839	LEU
1	A	841	LYS
1	A	875	ARG
1	A	881	GLN
1	A	888	LEU
1	A	893	ARG
1	A	916	ASP
1	A	954	THR
1	A	970	THR
1	A	987	LYS
1	A	998	GLN
1	A	1010	HIS
1	B	12	HIS
1	B	13	LYS
1	B	68	GLN
1	B	73	LYS
1	B	98	ASN
1	B	148	ARG
1	B	196	LEU
1	B	219	ASN
1	B	243	ILE
1	B	273	GLU
1	B	280	ILE
1	B	302	GLU
1	B	316	LYS
1	B	319	SER
1	B	325	LYS
1	B	352	LEU
1	B	361	LYS
1	B	375	LEU
1	B	387	SER
1	B	402	ARG
1	B	409	LEU
1	B	410	ASN
1	B	425	LEU
1	B	431	LEU
1	B	439	ASN
1	B	444	GLU
1	B	471	ILE
1	B	490	GLU

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Mol	Chain	Res	Type
1	B	503	PHE
1	B	516	LEU
1	B	532	GLN
1	B	550	HIS
1	B	565	LYS
1	B	568	PHE
1	B	570	VAL
1	B	589	LYS
1	B	606	ASN
1	B	610	LYS
1	B	703	LYS
1	B	715	ASP
1	B	727	LEU
1	B	742	THR
1	B	744	ILE
1	B	753	ARG
1	B	765	GLU
1	B	799	GLU
1	B	813	LYS
1	B	831	ASN
1	B	840	ILE
1	B	843	GLU
1	B	865	LYS
1	B	881	GLN
1	B	889	GLN
1	B	903	THR
1	B	913	GLU
1	B	944	SER
1	B	968	LYS
1	B	1007	HIS
1	B	1008	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	12	HIS
1	A	68	GLN
1	A	79	GLN
1	A	105	ASN
1	A	149	ASN
1	A	173	GLN

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	204	GLN
1	A	213	GLN
1	A	233	ASN
1	A	234	ASN
1	A	271	GLN
1	A	283	GLN
1	A	376	ASN
1	A	407	GLN
1	A	410	ASN
1	A	479	GLN
1	A	480	GLN
1	A	485	HIS
1	A	491	GLN
1	A	500	ASN
1	A	555	ASN
1	A	613	ASN
1	A	616	ASN
1	A	633	GLN
1	A	637	GLN
1	A	649	ASN
1	A	662	GLN
1	A	694	ASN
1	A	720	GLN
1	A	729	HIS
1	A	731	ASN
1	A	780	GLN
1	A	831	ASN
1	A	870	HIS
1	A	889	GLN
1	A	892	ASN
1	A	900	ASN
1	A	922	GLN
1	A	927	ASN
1	A	936	GLN
1	A	943	ASN
1	A	952	GLN
1	A	998	GLN
1	A	1009	HIS
1	B	2	ASN
1	B	68	GLN
1	B	71	GLN

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Mol	Chain	Res	Type
1	B	98	ASN
1	B	105	ASN
1	B	111	ASN
1	B	173	GLN
1	B	213	GLN
1	B	214	GLN
1	B	219	ASN
1	B	234	ASN
1	B	259	GLN
1	B	283	GLN
1	B	309	GLN
1	B	439	ASN
1	B	479	GLN
1	B	485	HIS
1	B	511	GLN
1	B	532	GLN
1	B	541	ASN
1	B	550	HIS
1	B	594	GLN
1	B	613	ASN
1	B	616	ASN
1	B	637	GLN
1	B	649	ASN
1	B	662	GLN
1	B	780	GLN
1	B	786	GLN
1	B	834	GLN
1	B	870	HIS
1	B	881	GLN
1	B	912	ASN
1	B	927	ASN
1	B	943	ASN
1	B	975	GLN
1	B	1004	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	2100	2	28,29,29	1.45	5 (17%)	43,45,45	1.07	3 (6%)
3	ADP	A	1100	2	28,29,29	1.56	4 (14%)	43,45,45	1.07	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	2100	2	-	3/16/32/32	0/3/3/3
3	ADP	A	1100	2	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1100	ADP	C2-N1	4.11	1.41	1.33
3	B	2100	ADP	C2-N1	4.10	1.41	1.33
3	A	1100	ADP	C4-N3	3.69	1.41	1.34
3	B	2100	ADP	C4-N3	2.99	1.40	1.34
3	A	1100	ADP	C6-N1	2.42	1.42	1.35
3	B	2100	ADP	PB-O2B	-2.31	1.46	1.54
3	B	2100	ADP	O4'-C4'	-2.21	1.40	1.45
3	A	1100	ADP	PB-O2B	-2.13	1.46	1.54
3	B	2100	ADP	C6-N1	2.01	1.41	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1100	ADP	O3'-C3'-C4'	2.73	118.93	111.08
3	B	2100	ADP	O3'-C3'-C4'	2.51	118.29	111.08
3	B	2100	ADP	O3'-C3'-C2'	2.44	119.65	111.82
3	A	1100	ADP	O3'-C3'-C2'	2.17	118.77	111.82
3	B	2100	ADP	O2'-C2'-C1'	2.04	117.12	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

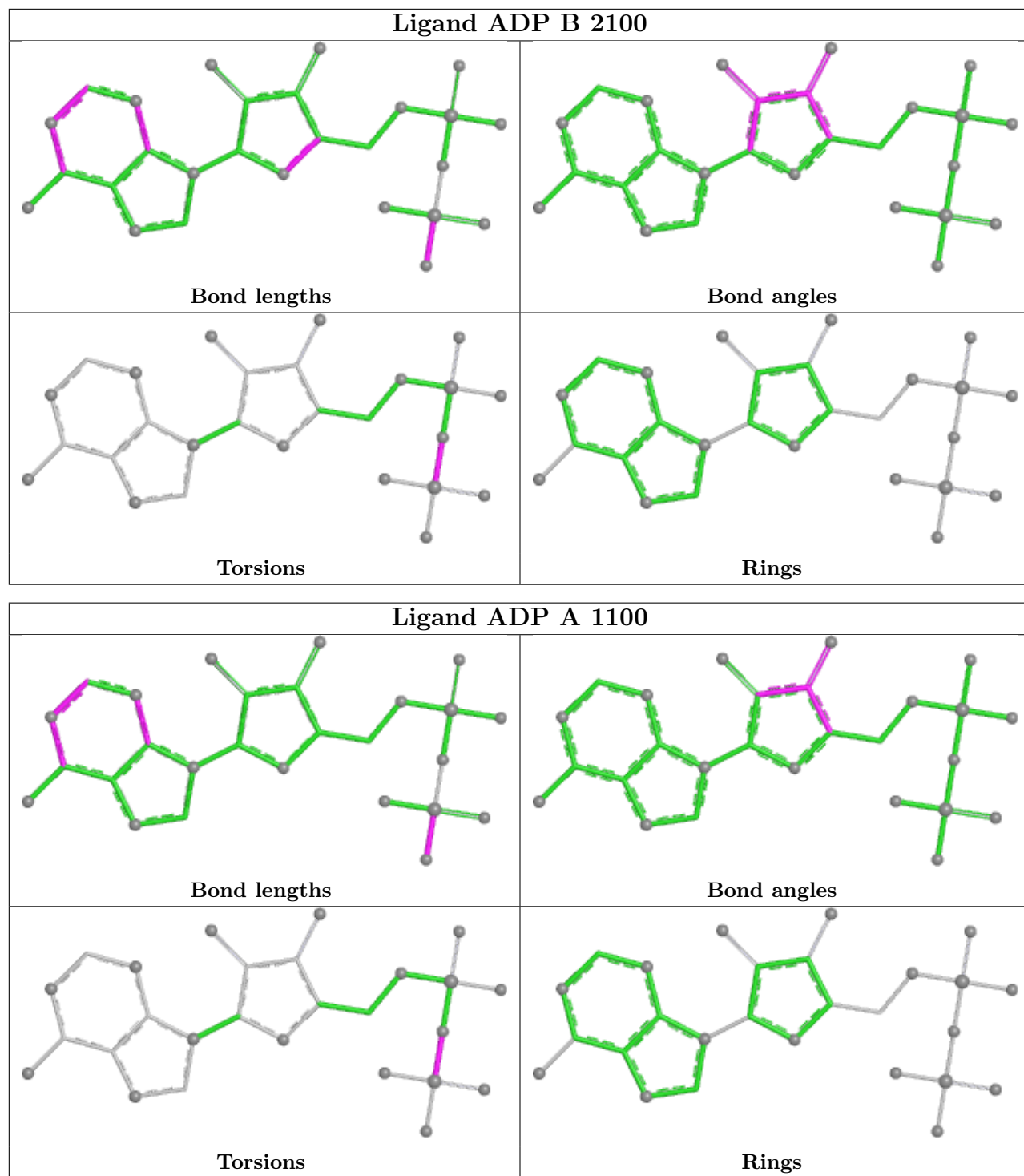
Mol	Chain	Res	Type	Atoms
3	A	1100	ADP	PA-O3A-PB-O2B
3	B	2100	ADP	PA-O3A-PB-O2B
3	A	1100	ADP	PA-O3A-PB-O1B
3	B	2100	ADP	PA-O3A-PB-O1B
3	B	2100	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2100	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	446:LYS	C	447:ALA	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1009/1010 (99%)	0.25	70 (6%) 23 16	17, 47, 100, 122	0
1	B	1009/1010 (99%)	0.30	58 (5%) 29 22	18, 50, 91, 118	0
All	All	2018/2020 (99%)	0.27	128 (6%) 26 19	17, 49, 96, 122	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	ILE	6.6
1	A	918	ILE	5.7
1	B	504	ILE	5.4
1	B	22	SER	5.3
1	A	1010	HIS	5.2
1	A	1007	HIS	5.1
1	A	1003	LEU	4.9
1	B	24	LEU	4.7
1	B	507	GLY	4.7
1	B	503	PHE	4.5
1	A	999	LYS	4.5
1	B	29	VAL	4.4
1	B	27	LEU	4.4
1	B	25	PHE	4.4
1	A	27	LEU	4.4
1	B	1010	HIS	4.4
1	A	1008	HIS	4.3
1	B	625	ALA	4.2
1	B	57	SER	4.2
1	A	29	VAL	4.2
1	A	921	VAL	4.2
1	A	22	SER	4.1
1	A	21	ASP	4.1
1	A	400	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	920	ALA	4.0
1	B	28	THR	4.0
1	B	20	GLY	4.0
1	A	28	THR	3.9
1	A	24	LEU	3.9
1	A	919	THR	3.8
1	A	995	GLU	3.8
1	B	23	ASP	3.8
1	A	535	PHE	3.8
1	B	506	PHE	3.6
1	A	922	GLN	3.5
1	B	1003	LEU	3.5
1	A	994	LEU	3.5
1	A	1005	HIS	3.5
1	B	26	LYS	3.4
1	B	207	GLY	3.3
1	B	363	ALA	3.3
1	B	209	GLY	3.3
1	A	992	ALA	3.2
1	A	26	LYS	3.2
1	B	205	ALA	3.2
1	A	622	LYS	3.2
1	A	915	GLY	3.2
1	A	991	LEU	3.1
1	A	997	LEU	3.1
1	B	39	PRO	3.1
1	A	793	ASP	3.0
1	A	205	ALA	3.0
1	A	25	PHE	3.0
1	B	53	VAL	2.9
1	A	993	GLU	2.9
1	A	998	GLN	2.8
1	B	443	SER	2.8
1	A	20	GLY	2.8
1	B	840	ILE	2.7
1	A	911	SER	2.7
1	B	72	VAL	2.7
1	B	41	PRO	2.7
1	A	1004	HIS	2.6
1	B	444	GLU	2.6
1	B	208	SER	2.6
1	A	302	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1000	ILE	2.6
1	B	61	THR	2.6
1	A	908	TYR	2.5
1	A	979	VAL	2.5
1	B	505	ASP	2.5
1	A	209	GLY	2.5
1	A	404	LEU	2.5
1	A	1006	HIS	2.5
1	B	1004	HIS	2.5
1	A	1002	ASP	2.5
1	B	515	ASP	2.5
1	A	904	THR	2.5
1	B	400	ALA	2.5
1	B	502	THR	2.5
1	B	63	LYS	2.5
1	B	622	LYS	2.5
1	A	925	LEU	2.5
1	B	799	GLU	2.5
1	A	990	LEU	2.4
1	A	910	GLY	2.4
1	B	42	ASP	2.4
1	B	1009	HIS	2.4
1	A	916	ASP	2.4
1	A	963	GLU	2.4
1	A	23	ASP	2.3
1	A	917	SER	2.3
1	A	996	ARG	2.3
1	B	362	GLY	2.3
1	A	207	GLY	2.3
1	A	366	GLY	2.3
1	A	959	ASN	2.3
1	A	923	ALA	2.3
1	B	918	ILE	2.3
1	A	1009	HIS	2.2
1	B	54	SER	2.2
1	B	1008	HIS	2.2
1	B	624	GLY	2.2
1	A	707	LEU	2.2
1	B	621	ALA	2.2
1	B	204	GLN	2.2
1	A	621	ALA	2.1
1	A	1001	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	395	GLU	2.1
1	B	627	PHE	2.1
1	A	361	LYS	2.1
1	A	508	LEU	2.1
1	A	935	CYS	2.1
1	B	797	SER	2.1
1	B	962	PRO	2.1
1	B	508	LEU	2.1
1	A	626	ASN	2.0
1	A	875	ARG	2.0
1	A	398	ILE	2.0
1	B	58	ASP	2.0
1	A	924	LYS	2.0
1	A	204	GLN	2.0
1	B	401	GLY	2.0
1	B	563	PHE	2.0
1	B	960	GLY	2.0
1	A	973	ALA	2.0
1	B	985	THR	2.0
1	A	986	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	2101	1/1	0.97	0.11	23,23,23,23	0
3	ADP	B	2100	27/27	0.98	0.06	22,32,37,38	0
3	ADP	A	1100	27/27	0.99	0.05	17,27,34,36	0

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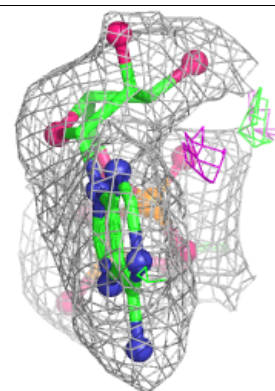
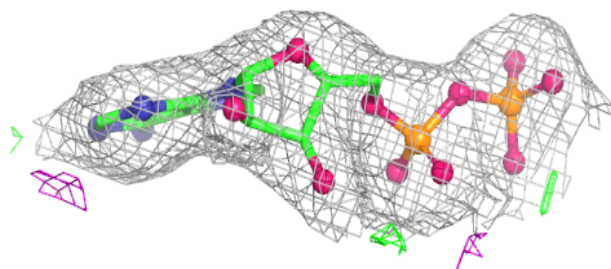
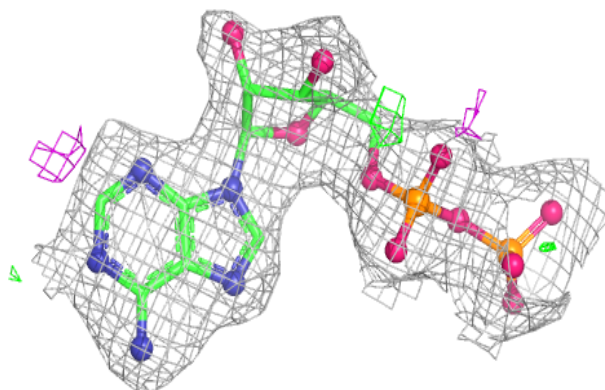
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1101	1/1	0.99	0.09	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

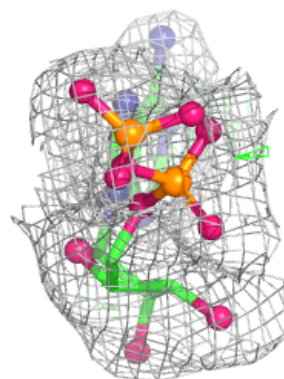
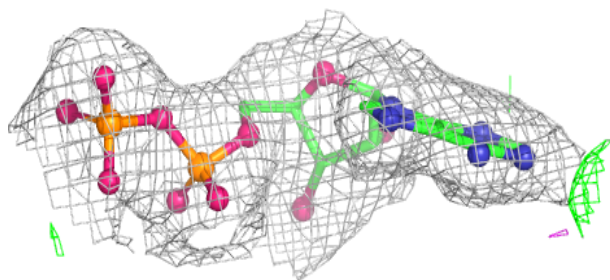
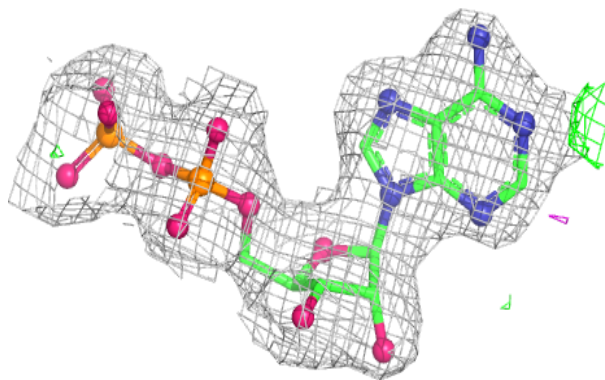
Electron density around ADP B 2100:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 1100:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.