



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 AM UTC

PDB ID : 1Q3R / pdb_00001q3r
Title : Crystal structure of the chaperonin from Thermococcus strain KS-1
(nucleotide-free form of single mutant)
Authors : Shomura, Y.; Yoshida, T.; Iizuka, R.; Maruyama, T.; Yohda, M.; Miki, K.
Deposited on : 2003-07-31
Resolution : 2.90 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
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

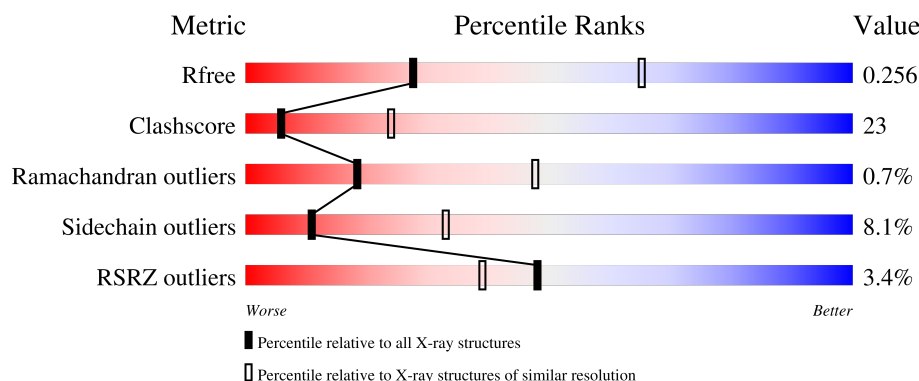
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	548	 3% 53% 38% 5%
1	B	548	 4% 56% 34% 5%
1	C	548	 3% 56% 33% 5% 5%
1	D	548	 3% 51% 37% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	4527	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15800 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.

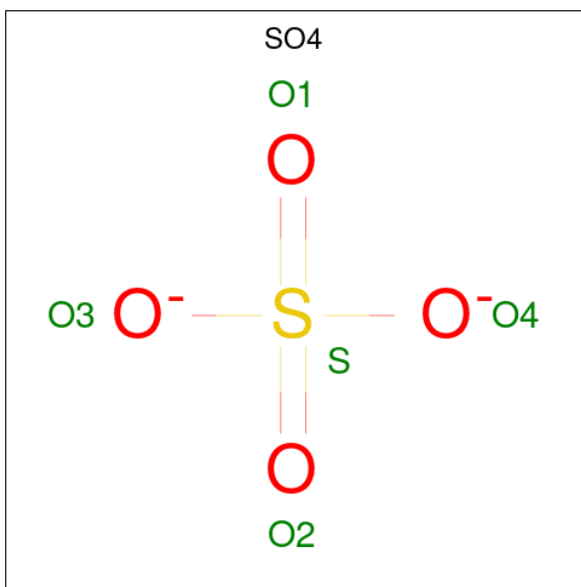
- Molecule 1 is a protein called Thermosome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3945	2484	673	772	16			
1	B	518	Total	C	N	O	S	0	0	0
			3945	2484	673	772	16			
1	C	518	Total	C	N	O	S	0	0	0
			3945	2484	673	772	16			
1	D	518	Total	C	N	O	S	0	0	0
			3945	2484	673	772	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	THR	ILE	engineered mutation	UNP O24729
B	125	THR	ILE	engineered mutation	UNP O24729
C	125	THR	ILE	engineered mutation	UNP O24729
D	125	THR	ILE	engineered mutation	UNP O24729

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

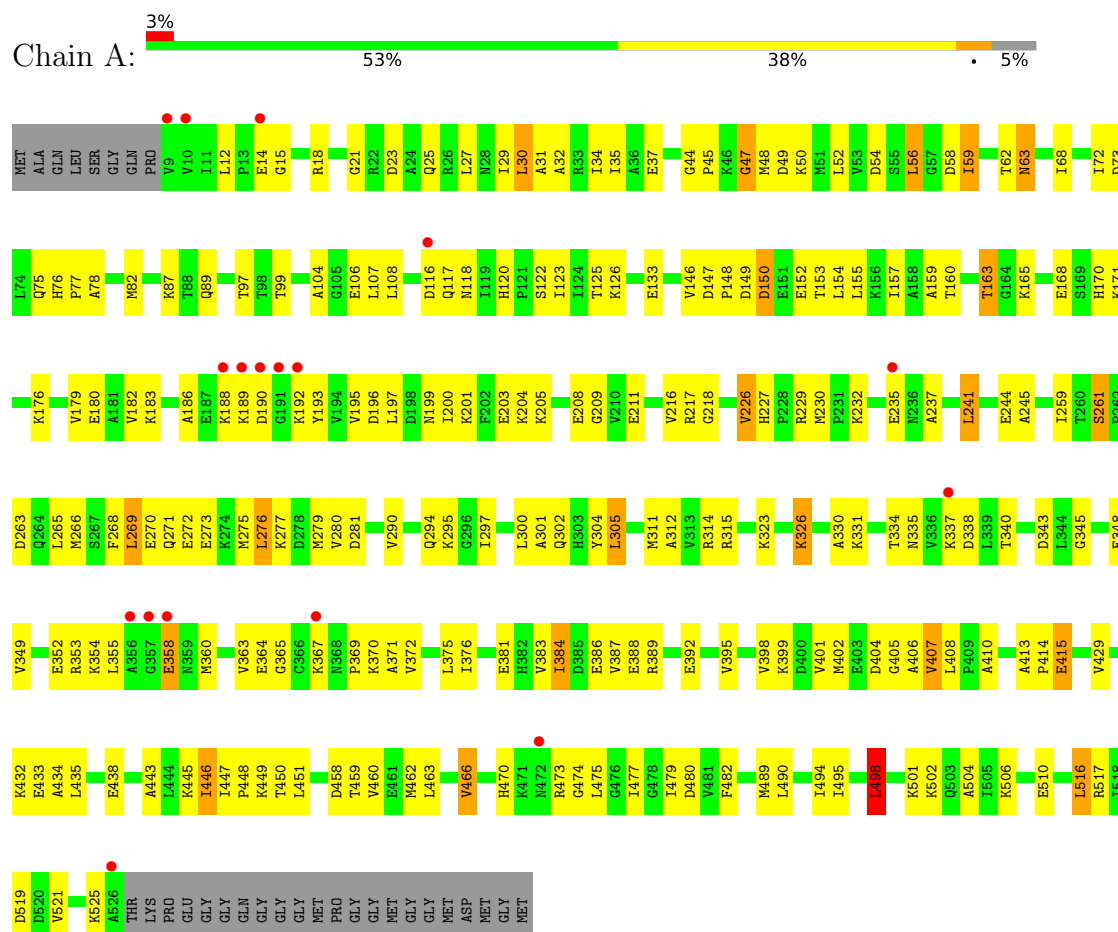


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

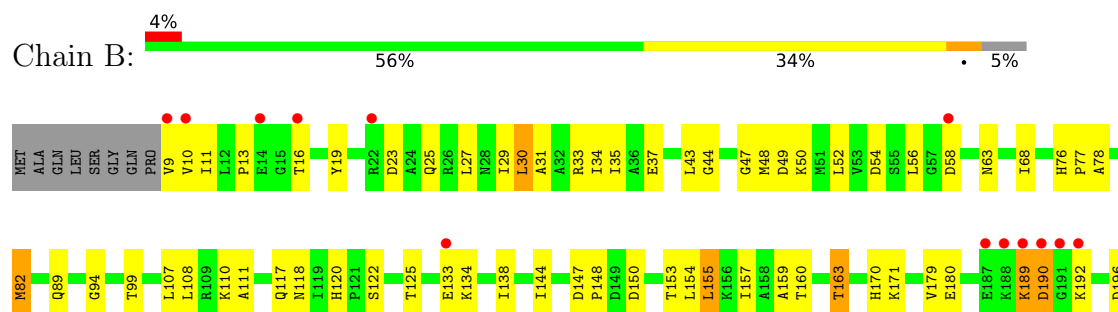
3 Residue-property plots

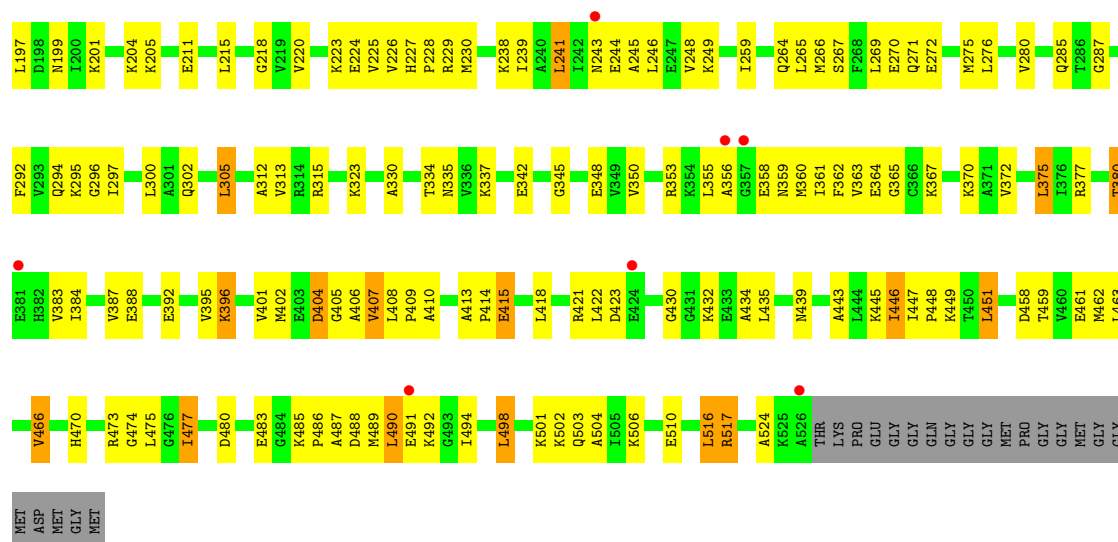
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Thermosome alpha subunit

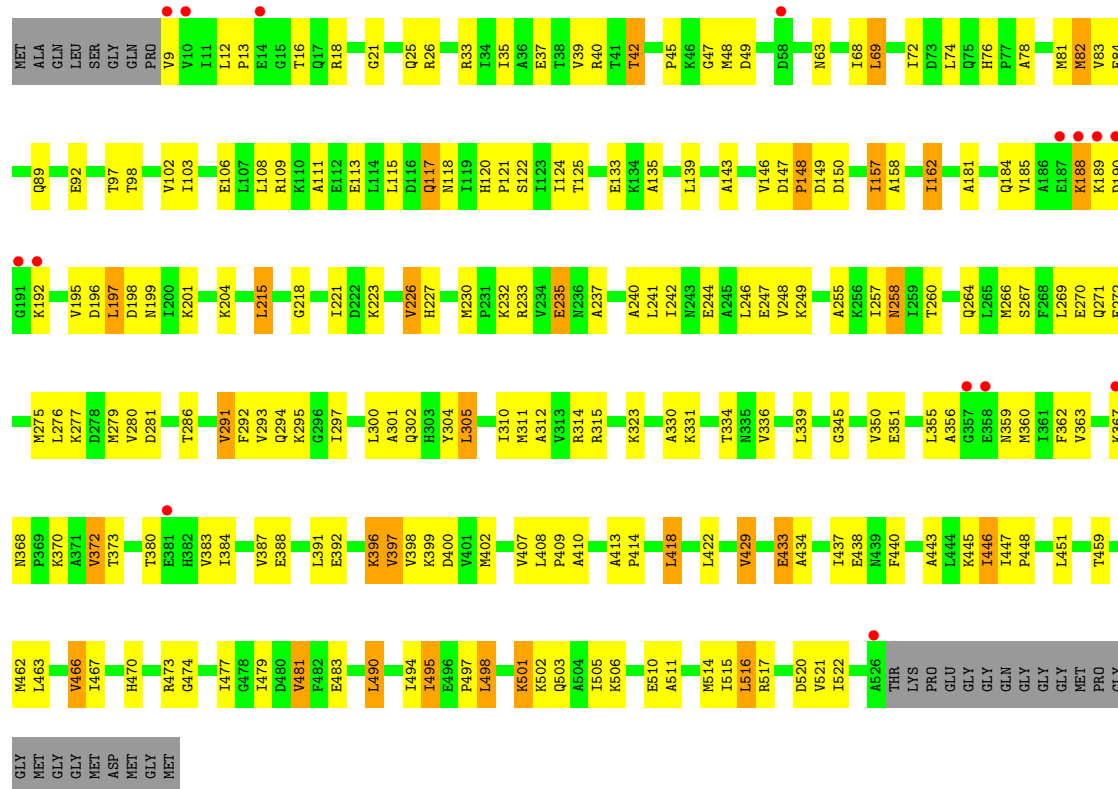


• Molecule 1: Thermosome alpha subunit



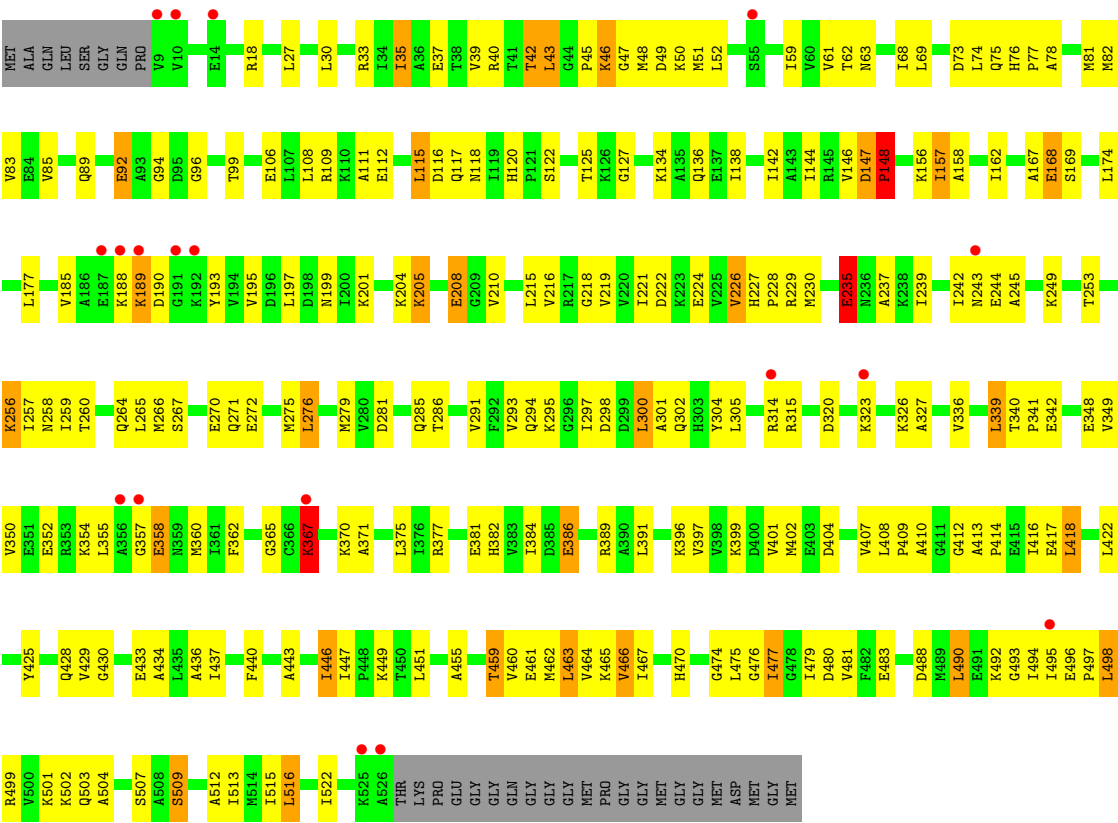


- Molecule 1: Thermosome alpha subunit



- Molecule 1: Thermosome alpha subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 210.06Å 157.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.94 – 2.90 93.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (93.94-2.90) 97.5 (93.94-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.257 0.212 , 0.256	Depositor DCC
R_{free} test set	3835 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15800	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: SO4

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	0.47	0/3980	0.95	13/5364 (0.2%)
1	B	0.47	0/3980	0.93	11/5364 (0.2%)
1	C	0.49	0/3980	0.98	11/5364 (0.2%)
1	D	0.46	0/3980	0.99	16/5364 (0.3%)
All	All	0.47	0/15920	0.96	51/21456 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	GLN	OE1-CD-NE2	-10.68	111.92	122.60
1	D	147	ASP	CA-C-N	9.79	132.07	119.84
1	D	147	ASP	C-N-CA	9.79	132.07	119.84
1	A	474	GLY	N-CA-C	8.69	120.90	112.04
1	C	474	GLY	N-CA-C	8.64	121.57	111.63
1	A	226	VAL	N-CA-C	8.17	119.93	110.62
1	B	239	ILE	N-CA-C	7.18	118.63	108.36
1	C	387	VAL	N-CA-C	-7.13	104.03	111.58
1	A	59	ILE	N-CA-C	6.91	117.84	108.17
1	A	63	ASN	N-CA-C	-6.90	104.53	114.12
1	D	239	ILE	N-CA-C	6.73	118.27	108.58
1	C	226	VAL	N-CA-C	6.71	118.27	110.62
1	A	44	GLY	CA-C-N	6.62	127.15	119.47
1	A	44	GLY	C-N-CA	6.62	127.15	119.47
1	B	44	GLY	CA-C-N	6.39	126.31	119.28
1	B	44	GLY	C-N-CA	6.39	126.31	119.28
1	C	113	GLU	N-CA-C	-6.25	104.54	111.36
1	B	226	VAL	N-CA-C	6.22	119.75	111.17
1	B	474	GLY	N-CA-C	6.14	120.54	111.76
1	C	117	GLN	CG-CD-NE2	6.13	125.60	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	LEU	N-CA-C	-6.12	104.68	111.36
1	B	475	LEU	N-CA-C	6.02	117.52	111.07
1	D	92	GLU	N-CA-C	5.99	117.61	111.14
1	C	473	ARG	N-CA-C	5.86	117.75	111.36
1	A	12	LEU	CA-C-N	5.83	125.59	119.76
1	A	12	LEU	C-N-CA	5.83	125.59	119.76
1	D	474	GLY	N-CA-C	5.78	122.98	112.58
1	D	237	ALA	N-CA-C	5.68	118.59	110.24
1	D	43	LEU	N-CA-C	5.64	118.63	110.28
1	D	117	GLN	N-CA-C	-5.58	106.45	113.20
1	D	440	PHE	N-CA-C	-5.54	105.24	111.28
1	D	59	ILE	N-CA-C	5.53	116.26	108.36
1	A	451	LEU	N-CA-C	-5.47	105.24	111.14
1	D	226	VAL	N-CA-C	5.42	117.82	111.05
1	D	327	ALA	N-CA-C	5.36	116.98	111.03
1	B	225	VAL	N-CA-C	-5.35	100.63	108.54
1	A	429	VAL	N-CA-C	-5.34	106.59	111.67
1	A	47	GLY	N-CA-C	-5.28	104.98	112.37
1	C	398	VAL	N-CA-C	-5.23	105.44	110.72
1	C	237	ALA	N-CA-C	5.22	117.88	110.10
1	B	421	ARG	N-CA-C	5.19	116.94	111.28
1	B	43	LEU	N-CA-C	5.15	117.77	110.10
1	A	237	ALA	N-CA-C	5.14	117.80	110.24
1	A	498	LEU	N-CA-C	-5.13	105.77	111.36
1	D	509	SER	N-CA-C	5.10	116.53	110.97
1	D	401	VAL	N-CA-C	5.09	115.87	110.72
1	D	208	GLU	CB-CA-C	-5.08	109.19	115.89
1	B	477	ILE	N-CA-C	5.06	115.52	108.84
1	C	440	PHE	N-CA-C	-5.06	105.68	111.14
1	C	286	THR	N-CA-C	-5.01	107.11	113.18
1	D	477	ILE	N-CA-C	5.01	115.46	108.84

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	3945	0	4125	186	0
1	B	3945	0	4125	181	0
1	C	3945	0	4125	198	0
1	D	3945	0	4125	213	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	2	0
All	All	15800	0	16500	742	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 23.

All (742) 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:C:503:GLN:HE22	1:D:208:GLU:H	1.05	1.02
1:D:201:LYS:HE3	1:D:323:LYS:HD2	1.41	1.02
1:C:272:GLU:HA	1:C:275:MET:HE2	1.43	0.99
1:D:33:ARG:HD3	1:D:109:ARG:HB2	1.43	0.99
1:D:157:ILE:HD12	1:D:495:ILE:HG23	1.46	0.98
1:D:370:LYS:HA	1:D:370:LYS:HE2	1.46	0.96
1:D:45:PRO:HG2	1:D:481:VAL:HG21	1.48	0.96
1:D:99:THR:HG23	2:D:4527:SO4:O1	1.67	0.94
1:C:188:LYS:HD3	1:C:188:LYS:H	1.31	0.94
1:D:271:GLN:HG3	1:D:275:MET:HE2	1.50	0.93
1:B:189:LYS:NZ	1:B:192:LYS:HB2	1.86	0.91
1:A:447:ILE:HB	1:A:448:PRO:HD3	1.53	0.89
1:C:396:LYS:HE3	1:C:399:LYS:HD3	1.54	0.88
1:C:157:ILE:HD12	1:C:495:ILE:HG23	1.57	0.87
1:C:92:GLU:HG2	1:C:503:GLN:HE21	1.39	0.86
1:C:503:GLN:HE22	1:D:208:GLU:N	1.73	0.85
1:B:159:ALA:O	1:B:163:THR:HG22	1.75	0.85
1:A:272:GLU:HA	1:A:275:MET:HE3	1.58	0.84
1:C:503:GLN:NE2	1:D:208:GLU:H	1.74	0.84
1:A:23:ASP:O	1:A:27:LEU:HD23	1.77	0.84
1:D:120:HIS:HD2	1:D:122:SER:H	1.24	0.84
1:C:157:ILE:HD12	1:C:495:ILE:CG2	2.09	0.83
1:C:68:ILE:O	1:C:72:ILE:HG22	1.79	0.83
1:D:112:GLU:HA	1:D:115:LEU:HD23	1.61	0.82
1:D:286:THR:HG21	1:D:339:LEU:HD13	1.61	0.81
1:B:189:LYS:HD3	1:B:189:LYS:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:HB2	1:A:193:TYR:CE2	2.16	0.81
1:A:462:MET:O	1:A:466:VAL:HG23	1.81	0.81
1:D:157:ILE:HG23	1:D:397:VAL:HG12	1.62	0.80
1:B:294:GLN:HE21	1:B:295:LYS:NZ	1.79	0.80
1:C:311:MET:HE1	1:C:350:VAL:HG12	1.63	0.80
1:C:157:ILE:HG23	1:C:397:VAL:HG13	1.63	0.80
1:D:227:HIS:HB3	1:D:230:MET:HG3	1.64	0.80
1:A:271:GLN:HG3	1:A:275:MET:HE2	1.65	0.79
1:B:204:LYS:HB2	1:B:384:ILE:HD12	1.64	0.79
1:C:84:GLU:CD	1:D:381:GLU:HG2	2.08	0.79
1:D:189:LYS:HE3	1:D:189:LYS:HA	1.65	0.78
1:D:201:LYS:CE	1:D:323:LYS:HD2	2.13	0.78
1:B:380:THR:HG22	1:B:383:VAL:H	1.47	0.78
1:A:62:THR:HG22	1:A:386:GLU:OE2	1.84	0.77
1:B:271:GLN:HG3	1:B:275:MET:HE2	1.66	0.77
1:B:157:ILE:HD11	1:B:407:VAL:CG2	2.14	0.77
1:B:462:MET:O	1:B:466:VAL:HG23	1.84	0.77
1:D:204:LYS:O	1:D:205:LYS:HE3	1.85	0.77
1:D:219:VAL:HG22	1:D:323:LYS:HE2	1.65	0.76
1:D:272:GLU:HA	1:D:275:MET:HE3	1.65	0.76
1:A:150:ASP:OD1	1:A:153:THR:HG23	1.84	0.76
1:B:227:HIS:HB3	1:B:230:MET:HG3	1.68	0.76
1:B:409:PRO:HB3	1:B:490:LEU:HD13	1.68	0.76
1:A:259:ILE:HD13	1:A:265:LEU:HD23	1.68	0.75
1:D:204:LYS:HB3	1:D:384:ILE:HD12	1.69	0.75
1:C:280:VAL:HG13	1:C:305:LEU:HD13	1.68	0.74
1:B:335:ASN:HB3	1:B:337:LYS:HG2	1.69	0.74
1:D:43:LEU:HD11	1:D:99:THR:HG22	1.70	0.73
1:A:280:VAL:HG13	1:A:305:LEU:HD13	1.69	0.73
1:C:45:PRO:HG2	1:C:481:VAL:HG21	1.69	0.73
1:B:447:ILE:HB	1:B:448:PRO:HD3	1.69	0.73
1:A:201:LYS:HB2	1:A:323:LYS:HE2	1.71	0.72
1:B:47:GLY:O	1:B:48:MET:HE2	1.89	0.72
1:C:397:VAL:HG22	1:C:497:PRO:HG2	1.70	0.72
1:A:76:HIS:HD2	1:A:78:ALA:H	1.35	0.72
1:B:150:ASP:OD1	1:B:153:THR:HG23	1.90	0.71
1:A:227:HIS:HB3	1:A:230:MET:HG3	1.71	0.71
1:C:355:LEU:HD22	1:C:360:MET:HE2	1.72	0.71
1:A:15:GLY:HA3	1:A:525:LYS:HD2	1.71	0.71
1:C:331:LYS:HD3	1:D:229:ARG:HE	1.54	0.71
1:C:443:ALA:O	1:C:446:ILE:HG13	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LEU:HD11	1:C:498:LEU:HD23	1.73	0.70
1:B:144:ILE:HD11	1:B:490:LEU:HD21	1.73	0.70
1:D:201:LYS:HE3	1:D:323:LYS:CD	2.19	0.70
1:D:413:ALA:HB3	1:D:414:PRO:HD3	1.73	0.70
1:D:222:ASP:OD1	1:D:360:MET:HE2	1.92	0.70
1:A:410:ALA:HB3	1:A:494:ILE:HG22	1.71	0.70
1:B:16:THR:HG22	1:B:524:ALA:HA	1.73	0.70
1:C:49:ASP:OD1	1:C:63:ASN:HB2	1.91	0.70
1:D:462:MET:O	1:D:466:VAL:HG22	1.92	0.69
1:D:340:THR:HG23	1:D:341:PRO:HD2	1.74	0.69
1:C:413:ALA:HB3	1:C:414:PRO:HD3	1.74	0.69
1:C:247:GLU:HA	1:C:276:LEU:HD11	1.75	0.69
1:B:266:MET:HE2	1:B:266:MET:HA	1.73	0.69
1:C:227:HIS:HB3	1:C:230:MET:HG3	1.74	0.68
1:D:410:ALA:HB3	1:D:494:ILE:HG22	1.75	0.68
1:B:82:MET:HE3	1:B:82:MET:HA	1.75	0.68
1:B:449:LYS:HG3	1:B:459:THR:HG23	1.75	0.68
1:C:388:GLU:O	1:C:392:GLU:HG3	1.93	0.68
1:D:39:VAL:O	1:D:42:THR:HG22	1.94	0.68
1:A:189:LYS:HG3	1:A:190:ASP:H	1.57	0.68
1:A:273:GLU:OE2	1:B:337:LYS:HE3	1.91	0.68
1:A:159:ALA:O	1:A:163:THR:HG22	1.93	0.68
1:D:120:HIS:CD2	1:D:122:SER:H	2.08	0.68
1:B:111:ALA:HB1	1:B:516:LEU:HD21	1.75	0.67
1:D:205:LYS:CD	1:D:360:MET:HE1	2.24	0.67
1:A:489:MET:HE2	1:A:489:MET:HA	1.75	0.67
1:C:82:MET:HE3	1:C:82:MET:HA	1.77	0.67
1:B:483:GLU:HG3	1:B:485:LYS:HE2	1.75	0.67
1:D:49:ASP:HB3	1:D:62:THR:O	1.95	0.67
1:C:266:MET:HE2	1:C:266:MET:HA	1.75	0.66
1:A:49:ASP:OD1	1:A:63:ASN:HB2	1.94	0.66
1:B:483:GLU:CG	1:B:485:LYS:HE2	2.25	0.66
1:D:340:THR:HG22	1:D:342:GLU:H	1.61	0.66
1:D:409:PRO:HA	1:D:495:ILE:HD12	1.75	0.66
1:A:326:LYS:HB3	1:A:371:ALA:HB2	1.75	0.66
1:D:266:MET:O	1:D:270:GLU:HG3	1.96	0.66
1:C:120:HIS:CD2	1:C:122:SER:H	2.12	0.66
1:B:498:LEU:HD13	1:B:502:LYS:HD2	1.77	0.66
1:B:517:ARG:HH11	1:B:517:ARG:HB3	1.61	0.66
1:A:73:ASP:O	1:B:13:PRO:HD3	1.95	0.66
1:A:87:LYS:O	1:A:87:LYS:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HG22	1:C:162:ILE:O	1.94	0.66
1:A:261:SER:HB2	1:A:263:ASP:OD2	1.96	0.66
1:B:241:LEU:HD22	1:B:330:ALA:HB3	1.78	0.65
1:C:230:MET:HE1	1:C:312:ALA:HB3	1.78	0.65
1:D:286:THR:HG21	1:D:339:LEU:CD1	2.26	0.65
1:B:111:ALA:CB	1:B:516:LEU:HD21	2.26	0.65
1:D:50:LYS:HD2	1:D:68:ILE:HD13	1.79	0.65
1:B:413:ALA:HB3	1:B:414:PRO:HD3	1.79	0.65
1:C:120:HIS:HD2	1:C:122:SER:H	1.44	0.65
1:C:409:PRO:HA	1:C:495:ILE:HD12	1.79	0.65
1:A:241:LEU:HD22	1:A:330:ALA:HB3	1.79	0.65
1:B:264:GLN:HA	1:B:267:SER:HB3	1.78	0.65
1:C:92:GLU:HG2	1:C:503:GLN:NE2	2.09	0.65
1:A:208:GLU:H	1:B:503:GLN:HE22	1.43	0.65
1:A:266:MET:HE3	1:B:275:MET:SD	2.37	0.65
1:B:23:ASP:O	1:B:27:LEU:HD23	1.97	0.65
1:C:271:GLN:O	1:C:275:MET:HG3	1.97	0.65
1:A:266:MET:O	1:A:270:GLU:HG3	1.96	0.64
1:C:198:ASP:O	1:C:323:LYS:HE3	1.97	0.64
1:D:205:LYS:HD2	1:D:360:MET:HE1	1.78	0.64
1:D:49:ASP:OD1	1:D:63:ASN:HB2	1.98	0.64
1:C:410:ALA:HB3	1:C:494:ILE:HG22	1.78	0.64
1:D:408:LEU:HD11	1:D:498:LEU:HD23	1.80	0.64
1:A:335:ASN:HB3	1:A:337:LYS:HG2	1.79	0.64
1:A:276:LEU:HD23	1:A:300:LEU:HB3	1.79	0.63
1:A:355:LEU:O	1:A:358:GLU:HG2	1.98	0.63
1:A:197:LEU:HD22	1:A:395:VAL:CG1	2.28	0.63
1:A:47:GLY:O	1:A:48:MET:HE2	1.98	0.63
1:B:243:ASN:O	1:B:295:LYS:HG2	1.99	0.63
1:A:434:ALA:O	1:A:438:GLU:HG3	1.99	0.63
1:C:359:ASN:O	1:C:360:MET:HG2	1.99	0.63
1:D:397:VAL:HG13	1:D:497:PRO:CG	2.29	0.63
1:B:49:ASP:OD1	1:B:63:ASN:HB2	1.98	0.62
1:C:13:PRO:HG3	1:D:75:GLN:NE2	2.13	0.62
1:B:445:LYS:O	1:B:448:PRO:HD2	1.99	0.62
1:A:330:ALA:HB2	1:A:345:GLY:HA3	1.82	0.62
1:D:407:VAL:HG22	1:D:495:ILE:HG13	1.80	0.62
1:A:498:LEU:HD22	1:A:502:LYS:HG3	1.80	0.62
1:D:43:LEU:CD1	1:D:99:THR:HG22	2.30	0.62
1:B:170:HIS:CD2	1:B:211:GLU:HG2	2.35	0.62
1:A:160:THR:HG21	1:A:494:ILE:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD22	1:B:395:VAL:HG12	1.82	0.61
1:B:388:GLU:O	1:B:392:GLU:HG3	2.00	0.61
1:D:157:ILE:CG2	1:D:397:VAL:HG12	2.30	0.61
1:D:177:LEU:HD22	1:D:215:LEU:HB2	1.81	0.61
1:B:230:MET:HE2	1:B:305:LEU:HB3	1.82	0.61
1:A:76:HIS:CD2	1:A:78:ALA:H	2.16	0.61
1:A:68:ILE:O	1:A:72:ILE:HG13	2.01	0.61
1:A:353:ARG:NH2	1:A:364:GLU:OE1	2.33	0.61
1:B:238:LYS:HD2	1:B:287:GLY:O	1.99	0.61
1:A:334:THR:HG22	1:A:335:ASN:ND2	2.16	0.61
1:B:259:ILE:HD13	1:B:265:LEU:HD23	1.82	0.61
1:C:45:PRO:HG2	1:C:481:VAL:CG2	2.30	0.61
1:C:506:LYS:O	1:C:510:GLU:HG3	2.01	0.61
1:B:197:LEU:HD22	1:B:395:VAL:CG1	2.31	0.61
1:B:266:MET:O	1:B:270:GLU:HG3	2.00	0.61
1:A:148:PRO:O	1:A:402:MET:HG2	2.01	0.61
1:A:408:LEU:HD11	1:A:498:LEU:HD23	1.82	0.61
1:C:102:VAL:HG12	1:C:446:ILE:HD13	1.82	0.61
1:C:409:PRO:HB3	1:C:490:LEU:HD13	1.82	0.60
1:A:294:GLN:HE21	1:A:295:LYS:NZ	1.98	0.60
1:D:157:ILE:CD1	1:D:495:ILE:HG23	2.27	0.60
1:C:81:MET:CE	1:C:515:ILE:HG12	2.31	0.60
1:D:466:VAL:HG11	1:D:479:ILE:HG13	1.82	0.60
1:B:480:ASP:OD1	1:B:492:LYS:HE2	2.02	0.60
1:D:78:ALA:HA	1:D:81:MET:HG3	1.83	0.60
1:B:272:GLU:HA	1:B:275:MET:HE3	1.84	0.60
1:B:297:ILE:HG22	1:B:302:GLN:HG3	1.84	0.60
1:B:458:ASP:OD2	1:B:461:GLU:HG3	2.01	0.60
1:A:227:HIS:HD2	1:A:229:ARG:H	1.49	0.59
1:D:498:LEU:HD22	1:D:502:LYS:CG	2.32	0.59
1:D:205:LYS:HG2	1:D:355:LEU:HB3	1.84	0.59
1:D:76:HIS:CD2	1:D:78:ALA:HB3	2.38	0.59
1:A:189:LYS:HG3	1:A:190:ASP:OD2	2.03	0.59
1:D:89:GLN:HE22	1:D:503:GLN:HB3	1.67	0.59
1:B:201:LYS:HB2	1:B:323:LYS:HE2	1.85	0.59
1:B:404:ASP:O	1:B:406:ALA:N	2.34	0.59
1:C:380:THR:OG1	1:C:383:VAL:HG23	2.03	0.59
1:A:117:GLN:O	1:A:118:ASN:HB2	2.02	0.58
1:B:33:ARG:O	1:B:37:GLU:HG3	2.03	0.58
1:D:460:VAL:O	1:D:464:VAL:HG23	2.02	0.58
1:A:190:ASP:C	1:A:192:LYS:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ALA:HB2	1:B:345:GLY:HA3	1.85	0.58
1:C:230:MET:HE2	1:C:310:ILE:O	2.03	0.58
1:B:54:ASP:OD2	1:B:58:ASP:HB3	2.03	0.58
1:B:157:ILE:HG13	1:B:401:VAL:HG21	1.85	0.58
1:B:241:LEU:HD12	1:B:292:PHE:HB2	1.86	0.58
1:C:277:LYS:HE2	1:C:281:ASP:OD2	2.03	0.58
1:A:21:GLY:O	1:A:25:GLN:HG3	2.04	0.58
1:C:197:LEU:CD1	1:C:399:LYS:HD2	2.34	0.58
1:A:193:TYR:HB2	1:A:402:MET:O	2.04	0.57
1:C:397:VAL:HG22	1:C:497:PRO:CG	2.33	0.57
1:A:157:ILE:HD11	1:A:407:VAL:HG22	1.85	0.57
1:B:271:GLN:HG3	1:B:275:MET:CE	2.34	0.57
1:C:157:ILE:CD1	1:C:495:ILE:HG23	2.31	0.57
1:A:30:LEU:HD13	1:B:9:VAL:HG13	1.86	0.57
1:B:52:LEU:HD11	1:B:68:ILE:HA	1.85	0.57
1:C:433:GLU:O	1:C:437:ILE:HG13	2.05	0.57
1:D:136:GLN:NE2	1:D:502:LYS:HD2	2.19	0.57
1:D:224:GLU:HB2	1:D:352:GLU:OE1	2.04	0.57
1:C:197:LEU:HD13	1:C:399:LYS:HD2	1.85	0.57
1:A:189:LYS:HG3	1:A:190:ASP:N	2.19	0.57
1:D:136:GLN:HE22	1:D:502:LYS:HD2	1.68	0.57
1:B:276:LEU:HD23	1:B:300:LEU:HB3	1.86	0.57
1:A:82:MET:HE1	1:A:104:ALA:HB3	1.86	0.57
1:C:84:GLU:OE1	1:D:381:GLU:HG2	2.04	0.57
1:D:281:ASP:O	1:D:285:GLN:HG3	2.04	0.57
1:A:381:GLU:OE2	1:A:381:GLU:N	2.38	0.57
1:A:383:VAL:O	1:A:387:VAL:HG23	2.05	0.57
1:B:223:LYS:HE3	1:B:315:ARG:O	2.05	0.57
1:A:160:THR:O	1:A:163:THR:HG23	2.05	0.56
1:C:18:ARG:HG3	1:C:522:ILE:HG12	1.87	0.56
1:D:106:GLU:HB2	1:D:446:ILE:HG12	1.86	0.56
1:D:245:ALA:HB2	1:D:295:LYS:HB3	1.87	0.56
1:A:163:THR:HB	1:A:171:LYS:NZ	2.20	0.56
1:B:449:LYS:HG3	1:B:459:THR:CG2	2.35	0.56
1:B:498:LEU:HD22	1:B:502:LYS:HG3	1.86	0.56
1:C:76:HIS:CD2	1:C:78:ALA:H	2.23	0.56
1:A:146:VAL:HG22	1:A:147:ASP:N	2.20	0.56
1:A:348:GLU:HB3	1:A:365:GLY:HA3	1.87	0.56
1:C:258:ASN:HB2	1:D:258:ASN:HD21	1.69	0.56
1:C:463:LEU:O	1:C:467:ILE:HG12	2.04	0.56
1:D:480:ASP:OD2	1:D:483:GLU:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:LEU:HD12	1:C:495:ILE:HD11	1.87	0.56
1:C:196:ASP:HB3	1:C:199:ASN:ND2	2.20	0.56
1:D:219:VAL:HG13	1:D:323:LYS:HD3	1.87	0.56
1:D:276:LEU:CD1	1:D:301:ALA:HB2	2.35	0.56
1:A:157:ILE:HD13	1:A:495:ILE:HG13	1.87	0.56
1:D:157:ILE:HG23	1:D:397:VAL:CG1	2.32	0.56
1:C:157:ILE:CG2	1:C:397:VAL:HG13	2.36	0.56
1:C:311:MET:HE1	1:C:350:VAL:CG1	2.33	0.55
1:B:25:GLN:O	1:B:29:ILE:HG12	2.06	0.55
1:C:271:GLN:HA	1:C:271:GLN:HE21	1.69	0.55
1:C:266:MET:O	1:C:270:GLU:HG3	2.06	0.55
1:A:415:GLU:HG3	1:A:447:ILE:HB	1.88	0.55
1:B:248:VAL:HG21	1:B:272:GLU:HB3	1.88	0.55
1:D:82:MET:HE3	1:D:515:ILE:HD11	1.88	0.55
1:B:404:ASP:C	1:B:406:ALA:H	2.14	0.55
1:C:232:LYS:O	1:C:351:GLU:HB2	2.06	0.55
1:B:56:LEU:HD23	1:B:56:LEU:O	2.06	0.55
1:C:271:GLN:HA	1:C:271:GLN:NE2	2.22	0.55
1:D:47:GLY:O	1:D:48:MET:HE2	2.06	0.55
1:A:470:HIS:HA	1:A:477:ILE:HB	1.89	0.55
1:D:76:HIS:CD2	1:D:78:ALA:H	2.25	0.55
1:D:470:HIS:HA	1:D:477:ILE:HB	1.89	0.55
1:A:32:ALA:O	1:A:35:ILE:HG22	2.07	0.55
1:B:196:ASP:HB3	1:B:199:ASN:ND2	2.22	0.54
1:D:446:ILE:HD12	1:D:446:ILE:H	1.73	0.54
1:B:488:ASP:CG	1:B:491:GLU:HG3	2.32	0.54
1:B:443:ALA:O	1:B:446:ILE:HG13	2.06	0.54
1:D:461:GLU:O	1:D:465:LYS:HD3	2.06	0.54
1:B:489:MET:HE2	1:B:489:MET:HA	1.89	0.54
1:A:176:LYS:O	1:A:180:GLU:HB2	2.08	0.54
1:C:258:ASN:HD22	1:D:258:ASN:ND2	2.05	0.54
1:A:445:LYS:O	1:A:448:PRO:HD2	2.07	0.54
1:D:127:GLY:HA3	1:D:436:ALA:HB3	1.88	0.54
1:B:160:THR:O	1:B:163:THR:HG23	2.08	0.54
1:B:243:ASN:OD1	1:B:334:THR:HA	2.07	0.54
1:C:195:VAL:HB	1:C:399:LYS:HG3	1.89	0.54
1:D:111:ALA:CB	1:D:516:LEU:HD21	2.38	0.54
1:A:75:GLN:NE2	1:B:13:PRO:HG3	2.23	0.54
1:D:227:HIS:HB3	1:D:230:MET:CG	2.37	0.54
1:D:397:VAL:HG13	1:D:497:PRO:HG2	1.89	0.54
1:A:386:GLU:OE2	1:A:386:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD22	1:B:34:ILE:HD11	1.90	0.53
1:B:498:LEU:CD1	1:B:502:LYS:HD2	2.37	0.53
1:C:111:ALA:CB	1:C:516:LEU:HD21	2.38	0.53
1:C:190:ASP:C	1:C:192:LYS:H	2.16	0.53
1:C:255:ALA:CB	1:D:257:ILE:HB	2.39	0.53
1:C:255:ALA:HB2	1:D:257:ILE:HB	1.89	0.53
1:D:157:ILE:HG22	1:D:158:ALA:N	2.23	0.53
1:C:42:THR:HG22	1:C:98:THR:HG21	1.90	0.53
1:C:201:LYS:HG2	1:C:323:LYS:HE2	1.89	0.53
1:C:396:LYS:O	1:C:396:LYS:HD3	2.08	0.53
1:D:386:GLU:OE2	1:D:389:ARG:HD2	2.07	0.53
1:A:76:HIS:HD2	1:A:78:ALA:N	2.05	0.53
1:D:272:GLU:CA	1:D:275:MET:HE3	2.38	0.53
1:D:300:LEU:HD22	1:D:304:TYR:CE2	2.42	0.53
1:C:115:LEU:HD13	1:C:124:ILE:HD12	1.89	0.53
1:C:188:LYS:H	1:C:188:LYS:CD	2.13	0.53
1:C:498:LEU:HD22	1:C:502:LYS:HG2	1.90	0.53
1:D:111:ALA:HB1	1:D:516:LEU:HD21	1.90	0.53
1:A:203:GLU:OE1	1:A:360:MET:HE1	2.09	0.53
1:B:94:GLY:CA	1:B:396:LYS:HG2	2.39	0.53
1:A:123:ILE:HG23	1:A:433:GLU:OE2	2.08	0.53
1:A:170:HIS:CD2	1:A:211:GLU:HG2	2.43	0.53
1:D:297:ILE:HG22	1:D:302:GLN:HG3	1.91	0.53
1:D:195:VAL:HB	1:D:399:LYS:HG3	1.91	0.53
1:A:446:ILE:O	1:A:450:THR:HG23	2.08	0.53
1:C:81:MET:HE1	1:C:515:ILE:HG12	1.91	0.53
1:D:51:MET:HG3	1:D:61:VAL:HG22	1.91	0.53
1:C:189:LYS:O	1:C:190:ASP:HB2	2.09	0.53
1:B:415:GLU:HG3	1:B:447:ILE:HB	1.91	0.52
1:D:271:GLN:HG3	1:D:275:MET:CE	2.32	0.52
1:D:350:VAL:HA	1:D:362:PHE:O	2.09	0.52
1:D:46:LYS:HG2	1:D:455:ALA:HA	1.92	0.52
1:B:144:ILE:CD1	1:B:490:LEU:HD21	2.38	0.52
1:B:409:PRO:HB3	1:B:490:LEU:CD1	2.39	0.52
1:C:204:LYS:HB2	1:C:384:ILE:HD12	1.91	0.52
1:D:266:MET:HE2	1:D:266:MET:HA	1.90	0.52
1:D:496:GLU:OE2	1:D:501:LYS:HE2	2.09	0.52
1:B:355:LEU:HD11	1:B:375:LEU:HD11	1.91	0.52
1:B:432:LYS:HA	1:B:435:LEU:HD13	1.90	0.52
1:D:449:LYS:HE2	1:D:459:THR:HG21	1.90	0.52
1:A:146:VAL:HG22	1:A:147:ASP:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLY:HA2	1:B:315:ARG:HD2	1.92	0.52
1:C:241:LEU:HD23	1:C:292:PHE:HB2	1.91	0.52
1:D:92:GLU:HG2	1:D:503:GLN:NE2	2.25	0.52
1:D:201:LYS:CD	1:D:323:LYS:HD2	2.40	0.52
1:A:99:THR:HG23	1:A:447:ILE:CD1	2.40	0.52
1:C:33:ARG:CZ	1:C:109:ARG:HG3	2.39	0.52
1:C:135:ALA:O	1:C:139:LEU:HG	2.10	0.52
1:C:264:GLN:HA	1:C:267:SER:OG	2.09	0.52
1:A:227:HIS:CD2	1:A:229:ARG:H	2.27	0.52
1:A:266:MET:HE2	1:A:269:LEU:HD23	1.92	0.52
1:C:143:ALA:HA	1:C:408:LEU:HD23	1.91	0.52
1:C:157:ILE:HG22	1:C:158:ALA:N	2.25	0.52
1:D:33:ARG:CD	1:D:109:ARG:HB2	2.29	0.52
1:D:446:ILE:HD12	1:D:446:ILE:N	2.25	0.52
1:C:188:LYS:HD3	1:C:188:LYS:N	2.13	0.51
1:A:208:GLU:N	1:B:503:GLN:HE22	2.07	0.51
1:A:190:ASP:C	1:A:192:LYS:N	2.68	0.51
1:A:123:ILE:HG21	1:A:432:LYS:HB2	1.91	0.51
1:A:37:GLU:CD	1:C:26:ARG:HH22	2.17	0.51
1:A:56:LEU:HD12	1:A:56:LEU:N	2.26	0.51
1:B:410:ALA:HB3	1:B:494:ILE:HG22	1.92	0.51
1:A:277:LYS:HE3	1:A:281:ASP:OD2	2.10	0.51
1:D:418:LEU:O	1:D:422:LEU:HG	2.11	0.51
1:D:490:LEU:CD1	1:D:495:ILE:HD13	2.41	0.51
1:A:204:LYS:HD3	1:A:388:GLU:CD	2.36	0.51
1:A:209:GLY:N	1:B:506:LYS:HD3	2.25	0.51
1:A:354:LYS:HE3	1:B:196:ASP:OD1	2.10	0.51
1:A:54:ASP:OD2	1:A:58:ASP:HB3	2.11	0.50
1:B:82:MET:HA	1:B:82:MET:CE	2.41	0.50
1:B:280:VAL:HG13	1:B:305:LEU:HD13	1.92	0.50
1:C:466:VAL:HG11	1:C:479:ILE:HG12	1.93	0.50
1:A:82:MET:HE1	1:A:104:ALA:CB	2.42	0.50
1:A:294:GLN:HE21	1:A:295:LYS:HZ3	1.58	0.50
1:C:13:PRO:HG3	1:D:75:GLN:CD	2.36	0.50
1:C:409:PRO:HB3	1:C:490:LEU:CD1	2.40	0.50
1:D:45:PRO:CG	1:D:481:VAL:HG21	2.31	0.50
1:D:242:ILE:O	1:D:293:VAL:HA	2.10	0.50
1:D:443:ALA:O	1:D:446:ILE:HG13	2.11	0.50
1:A:227:HIS:HB3	1:A:230:MET:CG	2.41	0.50
1:B:458:ASP:CG	1:B:461:GLU:HG3	2.36	0.50
1:C:47:GLY:C	1:C:48:MET:HE2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:MET:O	1:C:466:VAL:HG22	2.11	0.50
1:C:190:ASP:C	1:C:192:LYS:N	2.69	0.50
1:C:396:LYS:HD3	1:C:396:LYS:C	2.36	0.50
1:C:501:LYS:O	1:C:505:ILE:HG12	2.11	0.50
1:A:226:VAL:HG22	1:A:302:GLN:OE1	2.12	0.50
1:B:108:LEU:CD2	1:B:516:LEU:HD13	2.42	0.50
1:B:155:LEU:HD13	1:B:179:VAL:HG21	1.94	0.50
1:C:148:PRO:O	1:C:402:MET:HG2	2.12	0.50
1:B:47:GLY:C	1:B:48:MET:HE2	2.36	0.50
1:C:223:LYS:HE3	1:C:315:ARG:O	2.11	0.50
1:A:45:PRO:HB3	1:A:482:PHE:CE2	2.47	0.50
1:A:337:LYS:HG3	1:A:338:ASP:OD2	2.11	0.50
1:B:445:LYS:C	1:B:448:PRO:HD2	2.37	0.50
1:C:248:VAL:HG13	1:C:275:MET:CE	2.42	0.50
1:C:511:ALA:O	1:C:515:ILE:HG13	2.12	0.50
1:A:297:ILE:HG13	1:A:314:ARG:HB3	1.94	0.49
1:B:264:GLN:HA	1:B:267:SER:CB	2.41	0.49
1:B:488:ASP:O	1:B:492:LYS:HG3	2.11	0.49
1:C:147:ASP:O	1:C:149:ASP:N	2.45	0.49
1:C:215:LEU:HD21	1:C:372:VAL:HG11	1.94	0.49
1:A:208:GLU:H	1:B:503:GLN:NE2	2.09	0.49
1:B:218:GLY:HA3	1:B:363:VAL:O	2.12	0.49
1:B:439:ASN:N	1:B:439:ASN:HD22	2.09	0.49
1:C:106:GLU:HB2	1:C:446:ILE:HG12	1.93	0.49
1:A:201:LYS:HB2	1:A:323:LYS:CE	2.41	0.49
1:A:462:MET:CE	1:A:479:ILE:HG12	2.42	0.49
1:B:246:LEU:HD12	1:B:246:LEU:N	2.27	0.49
1:C:82:MET:HA	1:C:82:MET:CE	2.41	0.49
1:C:181:ALA:HB2	1:C:215:LEU:HD21	1.94	0.49
1:A:443:ALA:O	1:A:446:ILE:HG13	2.12	0.49
1:B:50:LYS:HD2	1:B:68:ILE:HD13	1.93	0.49
1:C:47:GLY:O	1:C:48:MET:HE2	2.13	0.49
1:D:185:VAL:CG1	1:D:199:ASN:HB2	2.43	0.49
1:A:126:LYS:HZ2	1:A:433:GLU:HG2	1.77	0.49
1:B:353:ARG:NH2	1:B:364:GLU:OE1	2.42	0.49
1:D:466:VAL:HG11	1:D:479:ILE:CG1	2.42	0.49
1:B:94:GLY:HA3	1:B:396:LYS:HG2	1.93	0.49
1:A:232:LYS:HD2	1:A:352:GLU:OE2	2.12	0.49
1:A:432:LYS:HA	1:A:435:LEU:HD13	1.95	0.49
1:A:376:ILE:HG22	1:A:384:ILE:HG12	1.95	0.49
1:B:367:LYS:HD3	1:B:367:LYS:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HZ3	1:C:323:LYS:NZ	2.09	0.48
1:D:188:LYS:HB3	1:D:193:TYR:CE2	2.48	0.48
1:D:340:THR:HG23	1:D:341:PRO:CD	2.40	0.48
1:B:76:HIS:HD2	1:B:78:ALA:HB3	1.78	0.48
1:C:81:MET:HE3	1:C:515:ILE:HG12	1.94	0.48
1:C:242:ILE:HD13	1:C:336:VAL:HG22	1.95	0.48
1:D:430:GLY:CA	1:D:434:ALA:HB2	2.43	0.48
1:A:269:LEU:HD21	1:B:249:LYS:HB2	1.95	0.48
1:B:294:GLN:HE21	1:B:295:LYS:HZ3	1.60	0.48
1:C:272:GLU:HA	1:C:275:MET:CE	2.30	0.48
1:A:106:GLU:HB2	1:A:446:ILE:HG12	1.95	0.48
1:A:196:ASP:HB3	1:A:199:ASN:ND2	2.29	0.48
1:A:218:GLY:HA3	1:A:363:VAL:O	2.12	0.48
1:A:462:MET:HE2	1:A:479:ILE:HG23	1.95	0.48
1:D:433:GLU:O	1:D:437:ILE:HG13	2.12	0.48
1:A:30:LEU:HD22	1:A:34:ILE:HD11	1.96	0.48
1:A:348:GLU:O	1:A:349:VAL:HG23	2.14	0.48
1:B:243:ASN:HA	1:B:294:GLN:HB3	1.94	0.48
1:D:120:HIS:HD2	1:D:122:SER:N	2.02	0.48
1:B:408:LEU:HD11	1:B:498:LEU:HD23	1.94	0.48
1:C:201:LYS:CG	1:C:323:LYS:HD2	2.43	0.48
1:D:205:LYS:HD3	1:D:360:MET:HE1	1.95	0.48
1:A:186:ALA:HA	1:A:195:VAL:HG22	1.96	0.48
1:A:204:LYS:HD2	1:A:384:ILE:HG23	1.95	0.48
1:C:201:LYS:HG2	1:C:323:LYS:CE	2.44	0.48
1:C:470:HIS:HA	1:C:477:ILE:HB	1.96	0.48
1:B:148:PRO:O	1:B:402:MET:HG2	2.14	0.47
1:B:294:GLN:HE21	1:B:295:LYS:HZ1	1.57	0.47
1:C:35:ILE:HD11	1:C:74:LEU:HD22	1.97	0.47
1:C:108:LEU:CD2	1:C:516:LEU:HD13	2.44	0.47
1:D:157:ILE:HD11	1:D:407:VAL:HG23	1.96	0.47
1:B:13:PRO:HD2	1:B:16:THR:HG21	1.96	0.47
1:C:201:LYS:HZ3	1:C:323:LYS:HZ2	1.60	0.47
1:C:244:GLU:OE1	1:C:336:VAL:HG23	2.14	0.47
1:C:514:MET:HE1	1:D:382:HIS:CB	2.43	0.47
1:D:77:PRO:O	1:D:81:MET:HG2	2.13	0.47
1:D:108:LEU:CD2	1:D:516:LEU:HD13	2.44	0.47
1:D:294:GLN:NE2	1:D:295:LYS:HE3	2.29	0.47
1:B:120:HIS:CE1	1:B:122:SER:HB2	2.49	0.47
1:B:201:LYS:HB2	1:B:323:LYS:CE	2.44	0.47
1:B:459:THR:O	1:B:463:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ILE:HG22	1:C:223:LYS:HB2	1.96	0.47
1:B:76:HIS:CD2	1:B:78:ALA:HB3	2.49	0.47
1:B:348:GLU:HB3	1:B:365:GLY:HA3	1.95	0.47
1:C:279:MET:HE2	1:C:336:VAL:HG21	1.95	0.47
1:D:447:ILE:O	1:D:451:LEU:HG	2.15	0.47
1:D:462:MET:CE	1:D:479:ILE:HG23	2.45	0.47
1:A:50:LYS:HD2	1:A:68:ILE:HD13	1.96	0.47
1:B:89:GLN:HE22	1:B:504:ALA:N	2.12	0.47
1:D:89:GLN:NE2	1:D:503:GLN:C	2.73	0.47
1:D:201:LYS:HG2	1:D:323:LYS:HD2	1.97	0.47
1:D:210:VAL:HA	1:D:377:ARG:O	2.14	0.47
1:D:294:GLN:O	1:D:315:ARG:HA	2.14	0.47
1:D:512:ALA:O	1:D:516:LEU:HB2	2.15	0.47
1:A:163:THR:HB	1:A:171:LYS:HZ2	1.79	0.47
1:C:257:ILE:HA	1:D:259:ILE:HB	1.95	0.47
1:C:294:GLN:HE21	1:C:295:LYS:NZ	2.13	0.47
1:C:521:VAL:HG13	1:D:51:MET:HE2	1.97	0.47
1:A:301:ALA:O	1:A:305:LEU:HD22	2.15	0.47
1:A:330:ALA:HB2	1:A:345:GLY:CA	2.44	0.47
1:A:458:ASP:C	1:A:458:ASP:OD2	2.58	0.47
1:C:240:ALA:HB3	1:C:291:VAL:HG13	1.96	0.47
1:D:37:GLU:O	1:D:40:ARG:HG2	2.15	0.47
1:D:89:GLN:NE2	1:D:504:ALA:N	2.62	0.47
1:A:18:ARG:HA	1:A:521:VAL:O	2.15	0.47
1:D:242:ILE:HD13	1:D:336:VAL:HG22	1.95	0.47
1:B:99:THR:HG23	1:B:447:ILE:CD1	2.45	0.47
1:B:227:HIS:HB3	1:B:230:MET:CG	2.43	0.47
1:C:201:LYS:HG3	1:C:323:LYS:HD2	1.95	0.47
1:D:463:LEU:O	1:D:467:ILE:HG13	2.15	0.47
1:D:148:PRO:O	1:D:402:MET:HG2	2.15	0.46
1:D:157:ILE:HD11	1:D:407:VAL:CG2	2.44	0.46
1:A:87:LYS:HD3	1:A:87:LYS:C	2.40	0.46
1:A:99:THR:HG23	1:A:447:ILE:HD12	1.96	0.46
1:A:197:LEU:HD22	1:A:395:VAL:HG12	1.95	0.46
1:A:498:LEU:HD13	1:A:502:LYS:HD2	1.97	0.46
1:D:215:LEU:C	1:D:215:LEU:HD13	2.40	0.46
1:A:245:ALA:HB2	1:A:295:LYS:HB3	1.97	0.46
1:C:368:ASN:C	1:C:368:ASN:HD22	2.21	0.46
1:D:221:ILE:HD12	1:D:320:ASP:HB3	1.97	0.46
1:A:297:ILE:HD12	1:A:314:ARG:HB3	1.97	0.46
1:B:227:HIS:CD2	1:B:229:ARG:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLN:O	1:C:118:ASN:HB2	2.14	0.46
1:C:233:ARG:NE	1:C:235:GLU:OE2	2.49	0.46
1:C:350:VAL:HA	1:C:362:PHE:O	2.16	0.46
1:D:157:ILE:CG2	1:D:158:ALA:N	2.79	0.46
1:A:335:ASN:CB	1:A:337:LYS:HG2	2.44	0.46
1:C:447:ILE:O	1:C:451:LEU:HG	2.15	0.46
1:A:275:MET:O	1:A:279:MET:HG3	2.16	0.46
1:A:297:ILE:CG1	1:A:314:ARG:HB3	2.45	0.46
1:B:163:THR:HB	1:B:171:LYS:CE	2.46	0.46
1:D:256:LYS:NZ	1:D:256:LYS:HB3	2.31	0.46
1:B:29:ILE:HG23	1:B:108:LEU:HB3	1.96	0.46
1:C:190:ASP:O	1:C:192:LYS:N	2.49	0.46
1:C:429:VAL:HG21	1:C:437:ILE:CD1	2.45	0.46
1:A:29:ILE:HG23	1:A:108:LEU:HB3	1.97	0.46
1:A:155:LEU:HA	1:A:179:VAL:HG21	1.97	0.46
1:B:189:LYS:HD3	1:B:189:LYS:N	2.24	0.46
1:B:446:ILE:HD12	1:B:447:ILE:H	1.81	0.46
1:C:115:LEU:HD11	1:C:121:PRO:HG3	1.97	0.46
1:C:157:ILE:HG23	1:C:397:VAL:CG1	2.41	0.46
1:C:429:VAL:HG21	1:C:437:ILE:HD12	1.98	0.46
1:D:108:LEU:HD22	1:D:516:LEU:HD13	1.98	0.46
1:D:226:VAL:HG12	1:D:314:ARG:HG2	1.96	0.46
1:D:227:HIS:CG	1:D:228:PRO:HD2	2.51	0.46
1:D:243:ASN:O	1:D:295:LYS:HD3	2.16	0.46
1:B:215:LEU:HD11	1:B:372:VAL:CG2	2.45	0.46
1:C:117:GLN:O	1:C:117:GLN:HG2	2.16	0.46
1:D:76:HIS:HD2	1:D:78:ALA:HB3	1.78	0.46
1:A:297:ILE:HG22	1:A:302:GLN:HG3	1.96	0.46
1:C:69:LEU:HB3	1:C:83:VAL:HG13	1.98	0.46
1:C:258:ASN:HD22	1:D:258:ASN:HD21	1.63	0.46
1:D:111:ALA:O	1:D:115:LEU:HD22	2.15	0.46
1:A:244:GLU:CD	1:A:335:ASN:HA	2.42	0.45
1:A:506:LYS:O	1:A:510:GLU:HG3	2.16	0.45
1:C:301:ALA:O	1:C:305:LEU:HD22	2.15	0.45
1:D:45:PRO:HG2	1:D:481:VAL:CG2	2.31	0.45
1:D:94:GLY:CA	1:D:396:LYS:HD2	2.46	0.45
1:A:62:THR:CG2	1:A:389:ARG:NE	2.79	0.45
1:B:19:TYR:N	1:B:19:TYR:CD1	2.85	0.45
1:C:33:ARG:HD3	1:C:109:ARG:HB2	1.98	0.45
1:B:245:ALA:HB2	1:B:295:LYS:HB2	1.98	0.45
1:D:146:VAL:HG22	1:D:147:ASP:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:HZ3	1:B:192:LYS:HB2	1.74	0.45
1:D:367:LYS:C	1:D:367:LYS:HE2	2.42	0.45
1:D:509:SER:O	1:D:513:ILE:HG13	2.17	0.45
1:A:462:MET:HE3	1:A:466:VAL:HG22	1.98	0.45
1:B:110:LYS:HB3	1:B:439:ASN:HB3	1.97	0.45
1:B:243:ASN:HA	1:B:294:GLN:CB	2.47	0.45
1:C:106:GLU:CB	1:C:446:ILE:HG12	2.45	0.45
1:D:162:ILE:HD13	1:D:174:LEU:HB2	1.98	0.45
1:D:409:PRO:HB3	1:D:490:LEU:HD22	1.98	0.45
1:B:76:HIS:HD2	1:B:78:ALA:H	1.65	0.45
1:C:33:ARG:NE	1:C:109:ARG:HG3	2.32	0.45
1:D:33:ARG:HD3	1:D:109:ARG:CB	2.30	0.45
1:B:117:GLN:O	1:B:118:ASN:HB2	2.17	0.45
1:B:447:ILE:O	1:B:451:LEU:HG	2.17	0.45
1:B:483:GLU:HG3	1:B:485:LYS:CE	2.46	0.45
1:C:76:HIS:HD2	1:C:78:ALA:H	1.63	0.45
1:C:227:HIS:HB3	1:C:230:MET:CG	2.43	0.45
1:C:275:MET:O	1:C:279:MET:HG3	2.17	0.45
1:C:280:VAL:HG11	1:C:304:TYR:HB2	1.99	0.45
1:D:340:THR:CG2	1:D:341:PRO:N	2.79	0.45
1:A:120:HIS:CE1	1:A:122:SER:HB2	2.52	0.45
1:C:517:ARG:HG2	1:C:517:ARG:HH11	1.81	0.45
1:D:18:ARG:HG3	1:D:522:ILE:HG12	1.98	0.45
1:D:85:VAL:HG13	1:D:507:SER:HB3	1.99	0.45
1:D:216:VAL:O	1:D:218:GLY:N	2.47	0.45
1:C:280:VAL:HG11	1:C:304:TYR:CB	2.47	0.45
1:A:447:ILE:HB	1:A:448:PRO:CD	2.36	0.44
1:B:415:GLU:CD	1:B:415:GLU:H	2.25	0.44
1:A:502:LYS:O	1:A:506:LYS:HG3	2.17	0.44
1:C:76:HIS:CD2	1:C:78:ALA:HB3	2.52	0.44
1:C:462:MET:HE2	1:C:479:ILE:HG23	1.98	0.44
1:D:244:GLU:HG3	1:D:249:LYS:NZ	2.32	0.44
1:D:462:MET:HE2	1:D:479:ILE:HG23	1.99	0.44
1:A:297:ILE:CD1	1:A:314:ARG:HB3	2.48	0.44
1:B:9:VAL:O	1:B:11:ILE:HG12	2.18	0.44
1:B:76:HIS:CD2	1:B:78:ALA:H	2.34	0.44
1:D:201:LYS:HB2	1:D:323:LYS:NZ	2.33	0.44
1:D:488:ASP:O	1:D:492:LYS:HG3	2.18	0.44
1:D:340:THR:HG22	1:D:341:PRO:N	2.31	0.44
1:D:348:GLU:O	1:D:349:VAL:HG23	2.18	0.44
1:B:313:VAL:HG21	1:B:361:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLU:OE2	1:B:342:GLU:N	2.49	0.44
1:C:226:VAL:CG1	1:C:314:ARG:HG2	2.48	0.44
1:C:226:VAL:HG12	1:C:314:ARG:HG2	1.98	0.44
1:C:410:ALA:HB3	1:C:494:ILE:CG2	2.45	0.44
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.83	0.44
1:A:498:LEU:HD13	1:A:502:LYS:CD	2.48	0.44
1:D:498:LEU:HD22	1:D:502:LYS:HG3	1.99	0.44
1:A:370:LYS:HA	1:A:370:LYS:HE3	2.00	0.44
1:B:506:LYS:O	1:B:510:GLU:HG3	2.18	0.44
1:C:37:GLU:HA	1:C:40:ARG:HG2	2.00	0.44
1:C:89:GLN:HG2	1:C:97:THR:HA	1.99	0.44
1:C:185:VAL:CG1	1:C:199:ASN:HB2	2.48	0.44
1:C:242:ILE:HG22	1:C:244:GLU:H	1.83	0.44
1:C:466:VAL:HG11	1:C:479:ILE:CG1	2.47	0.44
1:D:348:GLU:HB3	1:D:365:GLY:HA3	2.00	0.44
1:A:52:LEU:HD11	1:A:68:ILE:HA	2.00	0.44
1:C:330:ALA:HB2	1:C:345:GLY:HA3	2.00	0.44
1:D:279:MET:HE2	1:D:336:VAL:HG21	2.00	0.44
1:A:108:LEU:HD23	1:A:516:LEU:HD13	2.00	0.44
1:B:220:VAL:HG12	1:B:360:MET:HE2	2.00	0.44
1:A:208:GLU:HA	1:B:503:GLN:HE22	1.83	0.43
1:A:498:LEU:CD1	1:A:502:LYS:HD2	2.47	0.43
1:D:404:ASP:OD1	1:D:499:ARG:HB2	2.18	0.43
1:D:446:ILE:H	1:D:446:ILE:CD1	2.28	0.43
1:B:498:LEU:HD13	1:B:502:LYS:CD	2.46	0.43
1:C:516:LEU:HD12	1:C:516:LEU:HA	1.86	0.43
1:D:106:GLU:CB	1:D:446:ILE:HG12	2.49	0.43
1:B:189:LYS:HZ2	1:B:192:LYS:HB2	1.78	0.43
1:B:470:HIS:HA	1:B:477:ILE:HB	2.00	0.43
1:D:320:ASP:HA	1:D:323:LYS:HG2	2.01	0.43
1:A:388:GLU:O	1:A:392:GLU:HG3	2.18	0.43
1:C:115:LEU:HD13	1:C:124:ILE:CD1	2.48	0.43
1:C:297:ILE:HG22	1:C:302:GLN:HG3	2.01	0.43
1:A:217:ARG:HB3	1:A:369:PRO:HG3	2.00	0.43
1:A:280:VAL:HG11	1:A:304:TYR:HB3	2.00	0.43
1:B:117:GLN:O	1:B:117:GLN:HG2	2.18	0.43
1:B:355:LEU:HD22	1:B:377:ARG:CZ	2.48	0.43
1:B:383:VAL:O	1:B:387:VAL:HG23	2.18	0.43
1:C:248:VAL:HG13	1:C:275:MET:HE1	2.00	0.43
1:C:434:ALA:O	1:C:438:GLU:HG2	2.18	0.43
1:D:243:ASN:HA	1:D:294:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HA	1:A:163:THR:CG2	2.49	0.43
1:B:230:MET:HE1	1:B:312:ALA:HB3	1.99	0.43
1:D:230:MET:HE2	1:D:305:LEU:HB3	2.01	0.43
1:A:31:ALA:HB3	1:A:78:ALA:HB3	2.00	0.43
1:A:47:GLY:C	1:A:48:MET:HE2	2.42	0.43
1:B:244:GLU:HB3	1:B:334:THR:O	2.18	0.43
1:C:21:GLY:O	1:C:25:GLN:HG3	2.19	0.43
1:C:147:ASP:C	1:C:149:ASP:N	2.77	0.43
1:A:146:VAL:N	1:A:405:GLY:O	2.50	0.43
1:B:370:LYS:HE3	1:B:370:LYS:HA	2.01	0.43
1:C:33:ARG:CD	1:C:109:ARG:HG3	2.49	0.43
1:C:143:ALA:HA	1:C:408:LEU:CD2	2.47	0.43
1:D:235:GLU:O	1:D:348:GLU:O	2.36	0.43
1:B:189:LYS:HE2	1:B:189:LYS:HB2	1.77	0.43
1:D:354:LYS:O	1:D:355:LEU:HD12	2.18	0.43
1:A:404:ASP:C	1:A:406:ALA:H	2.27	0.43
1:A:446:ILE:HA	1:A:449:LYS:HB3	2.00	0.43
1:B:294:GLN:HE21	1:B:295:LYS:CE	2.32	0.43
1:B:380:THR:HG22	1:B:383:VAL:N	2.24	0.43
1:A:241:LEU:HD22	1:A:330:ALA:CB	2.48	0.42
1:B:418:LEU:O	1:B:422:LEU:HG	2.18	0.42
1:C:372:VAL:CG1	1:C:373:THR:N	2.80	0.42
1:C:446:ILE:HG13	1:C:446:ILE:H	1.54	0.42
1:D:52:LEU:HD11	1:D:68:ILE:HA	2.01	0.42
1:D:459:THR:HG22	1:D:460:VAL:N	2.33	0.42
1:A:30:LEU:HD21	1:C:26:ARG:HD3	2.00	0.42
1:C:82:MET:HE3	1:C:82:MET:CA	2.46	0.42
1:D:412:GLY:O	1:D:416:ILE:HG13	2.19	0.42
1:D:465:LYS:HD2	1:D:465:LYS:N	2.34	0.42
1:A:165:LYS:O	1:A:168:GLU:HG2	2.20	0.42
1:C:108:LEU:HD23	1:C:516:LEU:HD13	2.01	0.42
1:C:39:VAL:O	1:C:42:THR:HG22	2.20	0.42
1:D:106:GLU:HG2	1:D:446:ILE:HG13	2.01	0.42
1:A:106:GLU:OE2	1:A:446:ILE:HG23	2.20	0.42
1:A:182:VAL:HA	1:A:200:ILE:HD11	2.01	0.42
1:A:227:HIS:HB3	1:A:230:MET:SD	2.60	0.42
1:A:245:ALA:HB2	1:A:295:LYS:CB	2.49	0.42
1:A:268:PHE:O	1:A:272:GLU:HG3	2.19	0.42
1:A:415:GLU:CD	1:A:415:GLU:H	2.27	0.42
1:B:269:LEU:HD12	1:B:269:LEU:HA	1.89	0.42
1:D:134:LYS:O	1:D:138:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HG2	1:A:97:THR:HA	2.02	0.42
1:D:116:ASP:C	1:D:118:ASN:H	2.28	0.42
1:A:76:HIS:CD2	1:A:77:PRO:HD2	2.54	0.42
1:A:197:LEU:HG	1:A:399:LYS:HD2	2.01	0.42
1:B:227:HIS:HA	1:B:228:PRO:HD3	1.90	0.42
1:C:407:VAL:CG1	1:C:408:LEU:N	2.83	0.42
1:D:142:ILE:HD13	1:D:417:GLU:HG2	2.02	0.42
1:C:103:ILE:HA	1:C:446:ILE:HD11	2.02	0.42
1:C:244:GLU:CB	1:C:334:THR:O	2.68	0.42
1:D:249:LYS:HA	1:D:249:LYS:HD3	1.92	0.42
1:A:30:LEU:HD22	1:A:34:ILE:CD1	2.49	0.42
1:A:59:ILE:HD11	1:B:77:PRO:HA	2.02	0.42
1:A:226:VAL:HG12	1:A:312:ALA:O	2.20	0.42
1:C:520:ASP:HB3	1:D:50:LYS:HG2	2.02	0.42
1:D:167:ALA:O	1:D:168:GLU:C	2.62	0.42
1:A:413:ALA:HB3	1:A:414:PRO:HD3	2.02	0.42
1:B:29:ILE:HD12	1:B:108:LEU:HB3	2.02	0.42
1:C:13:PRO:HD3	1:D:73:ASP:O	2.20	0.42
1:C:355:LEU:O	1:C:356:ALA:C	2.63	0.42
1:D:156:LYS:HD3	1:D:493:GLY:HA2	2.01	0.42
1:D:264:GLN:O	1:D:265:LEU:C	2.61	0.42
1:A:334:THR:HG22	1:A:335:ASN:HD22	1.85	0.41
1:B:170:HIS:HD2	1:B:211:GLU:OE1	2.03	0.41
1:D:108:LEU:HD11	1:D:515:ILE:HD12	2.00	0.41
1:D:264:GLN:HA	1:D:267:SER:OG	2.20	0.41
1:A:182:VAL:HG11	1:A:398:VAL:HG12	2.01	0.41
1:B:197:LEU:CD2	1:B:395:VAL:HG12	2.50	0.41
1:B:473:ARG:HB2	1:B:477:ILE:HG13	2.02	0.41
1:D:340:THR:CG2	1:D:341:PRO:CD	2.98	0.41
1:D:352:GLU:HA	1:D:360:MET:O	2.20	0.41
1:B:189:LYS:HD3	1:B:192:LYS:O	2.20	0.41
1:C:33:ARG:HD3	1:C:109:ARG:CB	2.50	0.41
1:D:340:THR:CG2	1:D:341:PRO:HD2	2.48	0.41
1:D:476:GLY:HA2	1:D:490:LEU:CD2	2.50	0.41
1:C:372:VAL:HG13	1:C:373:THR:N	2.35	0.41
1:B:189:LYS:HE2	1:B:190:ASP:OD1	2.21	0.41
1:C:266:MET:CE	1:C:269:LEU:HD12	2.51	0.41
1:C:275:MET:SD	1:D:266:MET:HE3	2.61	0.41
1:C:293:VAL:HG12	1:C:295:LYS:H	1.85	0.41
1:B:430:GLY:CA	1:B:434:ALA:HB2	2.50	0.41
1:B:486:PRO:O	1:B:487:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:VAL:CG1	1:D:314:ARG:HG2	2.50	0.41
1:A:157:ILE:HD11	1:A:407:VAL:CG2	2.50	0.41
1:A:519:ASP:OD1	1:A:519:ASP:C	2.63	0.41
1:B:134:LYS:O	1:B:138:ILE:HG13	2.20	0.41
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.88	0.41
1:C:201:LYS:NZ	1:C:323:LYS:NZ	2.68	0.41
1:D:244:GLU:CD	1:D:249:LYS:HE3	2.46	0.41
1:A:216:VAL:O	1:A:218:GLY:N	2.51	0.41
1:B:31:ALA:HB3	1:B:78:ALA:HB3	2.03	0.41
1:C:331:LYS:HD3	1:D:229:ARG:NE	2.27	0.41
1:C:368:ASN:C	1:C:368:ASN:ND2	2.79	0.41
1:D:199:ASN:O	1:D:371:ALA:HA	2.21	0.41
1:D:425:TYR:O	1:D:428:GLN:HB2	2.20	0.41
1:A:89:GLN:HE22	1:A:504:ALA:N	2.19	0.41
1:A:149:ASP:OD2	1:A:193:TYR:HE1	2.03	0.41
1:A:179:VAL:O	1:A:183:LYS:HB2	2.21	0.41
1:A:190:ASP:O	1:A:192:LYS:N	2.54	0.41
1:A:205:LYS:HE3	1:A:360:MET:SD	2.61	0.41
1:A:290:VAL:HA	1:A:311:MET:O	2.21	0.41
1:B:82:MET:HE3	1:B:82:MET:CA	2.47	0.41
1:B:205:LYS:O	1:B:377:ARG:HD2	2.21	0.41
1:B:350:VAL:HA	1:B:362:PHE:O	2.21	0.41
1:C:9:VAL:HG12	1:D:27:LEU:HD22	2.02	0.41
1:C:147:ASP:HB3	1:C:150:ASP:HB2	2.01	0.41
1:C:189:LYS:HG3	1:C:190:ASP:OD1	2.21	0.41
1:C:195:VAL:O	1:C:399:LYS:HE2	2.20	0.41
1:D:74:LEU:HD12	1:D:83:VAL:CG2	2.51	0.41
1:D:430:GLY:HA2	1:D:434:ALA:HB2	2.03	0.41
1:B:30:LEU:HD22	1:B:34:ILE:CD1	2.51	0.41
1:B:180:GLU:OE2	1:B:215:LEU:HD23	2.21	0.41
1:B:224:GLU:HG2	1:B:359:ASN:HB3	2.03	0.41
1:D:96:GLY:HA2	2:D:4527:SO4:O1	2.21	0.41
1:D:118:ASN:HD22	1:D:118:ASN:HA	1.67	0.41
1:A:157:ILE:HG13	1:A:401:VAL:HG21	2.03	0.40
1:A:462:MET:O	1:A:466:VAL:CG2	2.61	0.40
1:B:355:LEU:O	1:B:356:ALA:C	2.63	0.40
1:C:218:GLY:HA3	1:C:363:VAL:O	2.21	0.40
1:D:35:ILE:HD11	1:D:74:LEU:HD22	2.03	0.40
1:A:340:THR:O	1:A:343:ASP:HB2	2.22	0.40
1:A:447:ILE:CB	1:A:448:PRO:HD3	2.37	0.40
1:A:473:ARG:HB2	1:A:477:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASP:OD2	1:A:480:ASP:C	2.64	0.40
1:B:108:LEU:HD23	1:B:516:LEU:HD13	2.02	0.40
1:B:330:ALA:HB2	1:B:345:GLY:CA	2.51	0.40
1:C:396:LYS:HE2	1:C:400:ASP:OD1	2.22	0.40
1:C:418:LEU:O	1:C:422:LEU:HG	2.21	0.40
1:C:498:LEU:HD22	1:C:502:LYS:CG	2.51	0.40
1:D:490:LEU:HD13	1:D:495:ILE:HD13	2.02	0.40
1:A:68:ILE:CG2	1:A:72:ILE:HD11	2.52	0.40
1:D:144:ILE:CD1	1:D:490:LEU:HD11	2.50	0.40
1:D:185:VAL:HG13	1:D:199:ASN:HB2	2.03	0.40
1:C:76:HIS:HD2	1:C:78:ALA:N	2.19	0.40
1:D:167:ALA:O	1:D:169:SER:N	2.54	0.40
1:D:189:LYS:O	1:D:190:ASP:HB2	2.20	0.40
1:D:358:GLU:CD	1:D:358:GLU:H	2.30	0.40
1:B:76:HIS:HA	1:B:77:PRO:HD3	1.93	0.40
1:B:205:LYS:NZ	1:B:358:GLU:HB2	2.37	0.40
1:C:12:LEU:HD13	1:C:16:THR:HG21	2.04	0.40
1:C:445:LYS:O	1:C:448:PRO:HG2	2.22	0.40
1:D:354:LYS:HE3	1:D:357:GLY:O	2.22	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	516/548 (94%)	497 (96%)	15 (3%)	4 (1%)	16	44
1	B	516/548 (94%)	502 (97%)	12 (2%)	2 (0%)	30	59
1	C	516/548 (94%)	489 (95%)	23 (4%)	4 (1%)	16	44
1	D	516/548 (94%)	492 (95%)	19 (4%)	5 (1%)	12	39
All	All	2064/2192 (94%)	1980 (96%)	69 (3%)	15 (1%)	18	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	367	LYS
1	A	475	LEU
1	D	235	GLU
1	C	235	GLU
1	D	148	PRO
1	D	367	LYS
1	A	150	ASP
1	C	367	LYS
1	D	475	LEU
1	B	405	GLY
1	C	162	ILE
1	D	168	GLU
1	B	10	VAL
1	C	148	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	422/440 (96%)	388 (92%)	34 (8%)	11	33
1	B	422/440 (96%)	393 (93%)	29 (7%)	14	41
1	C	422/440 (96%)	385 (91%)	37 (9%)	9	29
1	D	422/440 (96%)	386 (92%)	36 (8%)	10	31
All	All	1688/1760 (96%)	1552 (92%)	136 (8%)	11	33

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	30	LEU
1	A	56	LEU
1	A	107	LEU
1	A	116	ASP

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Mol	Chain	Res	Type
1	A	125	THR
1	A	133	GLU
1	A	152	GLU
1	A	154	LEU
1	A	163	THR
1	A	241	LEU
1	A	261	SER
1	A	269	LEU
1	A	276	LEU
1	A	305	LEU
1	A	315	ARG
1	A	326	LYS
1	A	331	LYS
1	A	358	GLU
1	A	372	VAL
1	A	375	LEU
1	A	384	ILE
1	A	407	VAL
1	A	415	GLU
1	A	446	ILE
1	A	459	THR
1	A	460	VAL
1	A	463	LEU
1	A	466	VAL
1	A	490	LEU
1	A	498	LEU
1	A	501	LYS
1	A	516	LEU
1	A	517	ARG
1	B	30	LEU
1	B	35	ILE
1	B	82	MET
1	B	107	LEU
1	B	125	THR
1	B	133	GLU
1	B	147	ASP
1	B	154	LEU
1	B	155	LEU
1	B	163	THR
1	B	189	LYS
1	B	190	ASP
1	B	241	LEU

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Mol	Chain	Res	Type
1	B	285	GLN
1	B	305	LEU
1	B	375	LEU
1	B	380	THR
1	B	396	LYS
1	B	404	ASP
1	B	407	VAL
1	B	415	GLU
1	B	423	ASP
1	B	446	ILE
1	B	466	VAL
1	B	490	LEU
1	B	498	LEU
1	B	501	LYS
1	B	516	LEU
1	B	517	ARG
1	C	42	THR
1	C	69	LEU
1	C	82	MET
1	C	125	THR
1	C	133	GLU
1	C	146	VAL
1	C	157	ILE
1	C	184	GLN
1	C	188	LYS
1	C	197	LEU
1	C	215	LEU
1	C	246	LEU
1	C	249	LYS
1	C	258	ASN
1	C	260	THR
1	C	291	VAL
1	C	300	LEU
1	C	305	LEU
1	C	339	LEU
1	C	370	LYS
1	C	372	VAL
1	C	391	LEU
1	C	396	LYS
1	C	397	VAL
1	C	418	LEU
1	C	429	VAL

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Mol	Chain	Res	Type
1	C	433	GLU
1	C	446	ILE
1	C	459	THR
1	C	466	VAL
1	C	481	VAL
1	C	483	GLU
1	C	490	LEU
1	C	495	ILE
1	C	498	LEU
1	C	501	LYS
1	C	516	LEU
1	D	30	LEU
1	D	35	ILE
1	D	42	THR
1	D	46	LYS
1	D	69	LEU
1	D	115	LEU
1	D	125	THR
1	D	148	PRO
1	D	157	ILE
1	D	189	LYS
1	D	197	LEU
1	D	205	LYS
1	D	235	GLU
1	D	253	THR
1	D	256	LYS
1	D	260	THR
1	D	276	LEU
1	D	291	VAL
1	D	298	ASP
1	D	300	LEU
1	D	326	LYS
1	D	339	LEU
1	D	358	GLU
1	D	367	LYS
1	D	375	LEU
1	D	386	GLU
1	D	391	LEU
1	D	418	LEU
1	D	429	VAL
1	D	446	ILE
1	D	459	THR

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Mol	Chain	Res	Type
1	D	463	LEU
1	D	466	VAL
1	D	490	LEU
1	D	498	LEU
1	D	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	25	GLN
1	A	28	ASN
1	A	76	HIS
1	A	89	GLN
1	A	118	ASN
1	A	170	HIS
1	A	199	ASN
1	A	227	HIS
1	A	236	ASN
1	A	285	GLN
1	A	294	GLN
1	A	335	ASN
1	A	368	ASN
1	A	472	ASN
1	A	503	GLN
1	B	28	ASN
1	B	75	GLN
1	B	76	HIS
1	B	89	GLN
1	B	117	GLN
1	B	118	ASN
1	B	170	HIS
1	B	184	GLN
1	B	199	ASN
1	B	227	HIS
1	B	294	GLN
1	B	439	ASN
1	B	503	GLN
1	C	25	GLN
1	C	28	ASN
1	C	76	HIS
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	118	ASN
1	C	120	HIS
1	C	136	GLN
1	C	258	ASN
1	C	271	GLN
1	C	285	GLN
1	C	294	GLN
1	C	303	HIS
1	C	335	ASN
1	C	368	ASN
1	C	503	GLN
1	D	28	ASN
1	D	76	HIS
1	D	89	GLN
1	D	117	GLN
1	D	118	ASN
1	D	120	HIS
1	D	136	GLN
1	D	236	ASN
1	D	258	ASN
1	D	271	GLN
1	D	285	GLN
1	D	302	GLN
1	D	368	ASN
1	D	382	HIS
1	D	439	ASN
1	D	503	GLN

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 [i](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	B	2527	-	4,4,4	0.35	0	6,6,6	0.16	0
2	SO4	D	4527	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	C	3527	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	A	1527	-	4,4,4	0.38	0	6,6,6	0.09	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4527	SO4	2	0

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

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	518/548 (94%)	-0.06	17 (3%) 49 40	7, 21, 37, 74	0
1	B	518/548 (94%)	-0.09	20 (3%) 43 35	8, 21, 37, 82	0
1	C	518/548 (94%)	-0.14	15 (2%) 53 45	5, 19, 37, 70	0
1	D	518/548 (94%)	-0.05	18 (3%) 47 38	5, 21, 37, 68	0
All	All	2072/2192 (94%)	-0.09	70 (3%) 48 39	5, 20, 37, 82	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	526	ALA	4.5
1	B	189	LYS	4.3
1	A	526	ALA	4.0
1	B	192	LYS	4.0
1	D	357	GLY	3.8
1	A	191	GLY	3.7
1	D	356	ALA	3.7
1	C	526	ALA	3.5
1	C	189	LYS	3.5
1	C	187	GLU	3.5
1	A	189	LYS	3.5
1	C	188	LYS	3.5
1	D	9	VAL	3.4
1	B	526	ALA	3.4
1	B	191	GLY	3.3
1	B	188	LYS	3.3
1	D	323	LYS	3.3
1	B	190	ASP	3.3
1	B	357	GLY	3.3
1	C	357	GLY	3.2
1	A	188	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	3.2
1	A	367	LYS	3.1
1	B	9	VAL	3.0
1	D	367	LYS	2.9
1	A	356	ALA	2.9
1	A	472	ASN	2.8
1	C	191	GLY	2.8
1	D	525	LYS	2.8
1	A	9	VAL	2.8
1	B	243	ASN	2.8
1	C	190	ASP	2.7
1	B	14	GLU	2.7
1	C	367	LYS	2.7
1	D	187	GLU	2.7
1	C	192	LYS	2.7
1	D	189	LYS	2.7
1	D	14	GLU	2.6
1	C	9	VAL	2.6
1	A	235	GLU	2.6
1	B	356	ALA	2.6
1	C	10	VAL	2.6
1	B	16	THR	2.5
1	D	55	SER	2.5
1	B	187	GLU	2.5
1	A	190	ASP	2.5
1	A	10	VAL	2.5
1	B	491	GLU	2.4
1	A	337	LYS	2.4
1	B	424	GLU	2.4
1	A	14	GLU	2.4
1	D	191	GLY	2.3
1	B	22	ARG	2.3
1	D	243	ASN	2.3
1	C	358	GLU	2.3
1	D	188	LYS	2.3
1	D	192	LYS	2.3
1	B	10	VAL	2.3
1	D	314	ARG	2.2
1	A	192	LYS	2.1
1	A	358	GLU	2.1
1	D	495	ILE	2.1
1	C	58	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	381	GLU	2.1
1	D	10	VAL	2.1
1	A	116	ASP	2.1
1	B	133	GLU	2.1
1	C	14	GLU	2.1
1	B	58	ASP	2.0
1	C	381	GLU	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	SO4	D	4527	5/5	0.89	0.17	37,37,37,37	0
2	SO4	C	3527	5/5	0.92	0.16	41,42,42,42	0
2	SO4	A	1527	5/5	0.94	0.11	42,43,43,43	0
2	SO4	B	2527	5/5	0.95	0.11	36,37,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.