



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:59 PM UTC

PDB ID : 1BXN / pdb_00001bxn
Title : THE CRYSTAL STRUCTURE OF RUBISCO FROM ALCALIGENES EUTROPHUS TO 2.7 ANGSTROMS.
Authors : Hansen, S.; Vollan, V.B.; Hough, E.; Andersen, K.
Deposited on : 1998-10-06
Resolution : 2.70 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

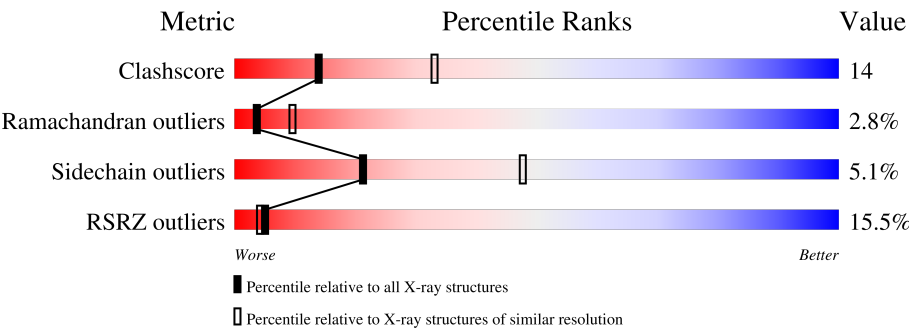
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	485	14% 62% 26% • 8%
1	C	485	11% 63% 26% • 8%
1	E	485	13% 63% 26% • 8%
1	G	485	14% 64% 25% • 8%
2	I	139	16% 54% 31% 7% • 7%
2	J	139	22% 53% 34% 6% • 7%
2	K	139	19% 53% 35% 5% • 7%

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Mol	Chain	Length	Quality of chain
2	L	139	19% 50% 35% 6% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18144 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 PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3470	2201	612	636	21			
1	C	445	Total	C	N	O	S	0	0	0
			3470	2201	612	636	21			
1	E	445	Total	C	N	O	S	0	0	0
			3470	2201	612	636	21			
1	G	445	Total	C	N	O	S	0	0	0
			3470	2201	612	636	21			

- Molecule 2 is a protein called PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	129	Total	C	N	O	S	0	0	0
			1056	670	180	200	6			
2	J	129	Total	C	N	O	S	0	0	0
			1056	670	180	200	6			
2	K	129	Total	C	N	O	S	0	0	0
			1056	670	180	200	6			
2	L	129	Total	C	N	O	S	0	0	0
			1056	670	180	200	6			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

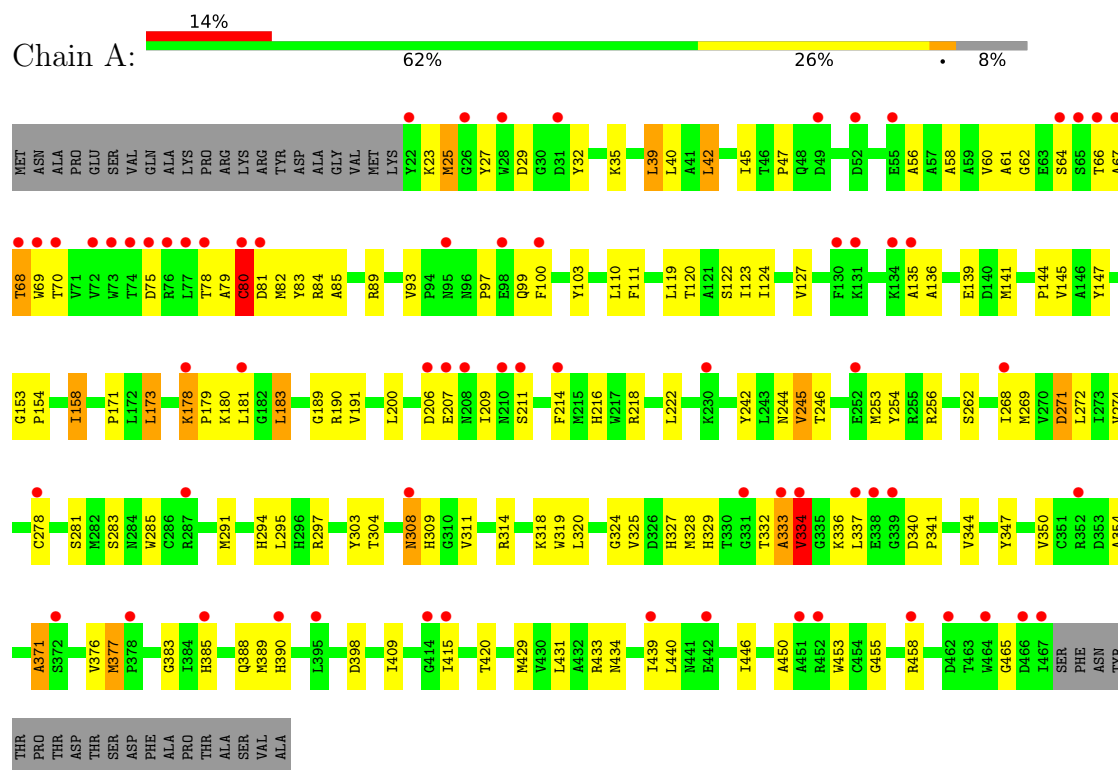


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

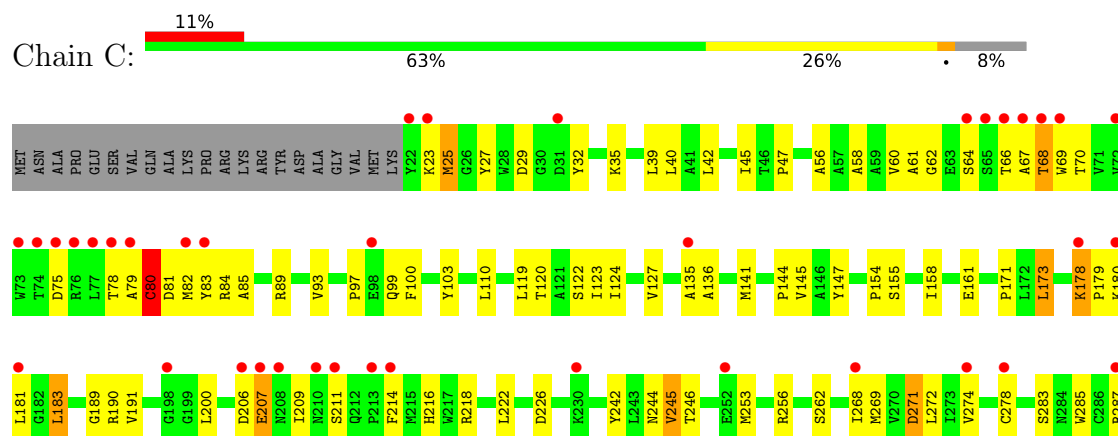
3 Residue-property plots

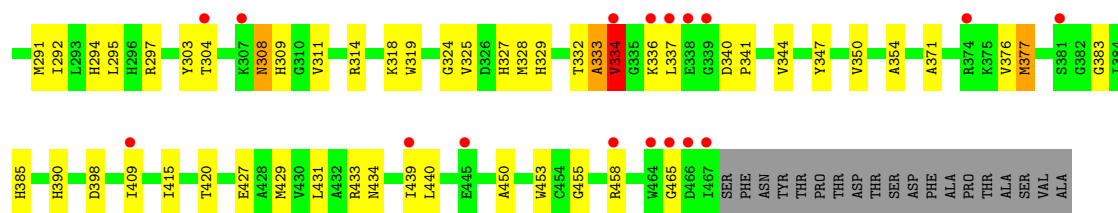
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)

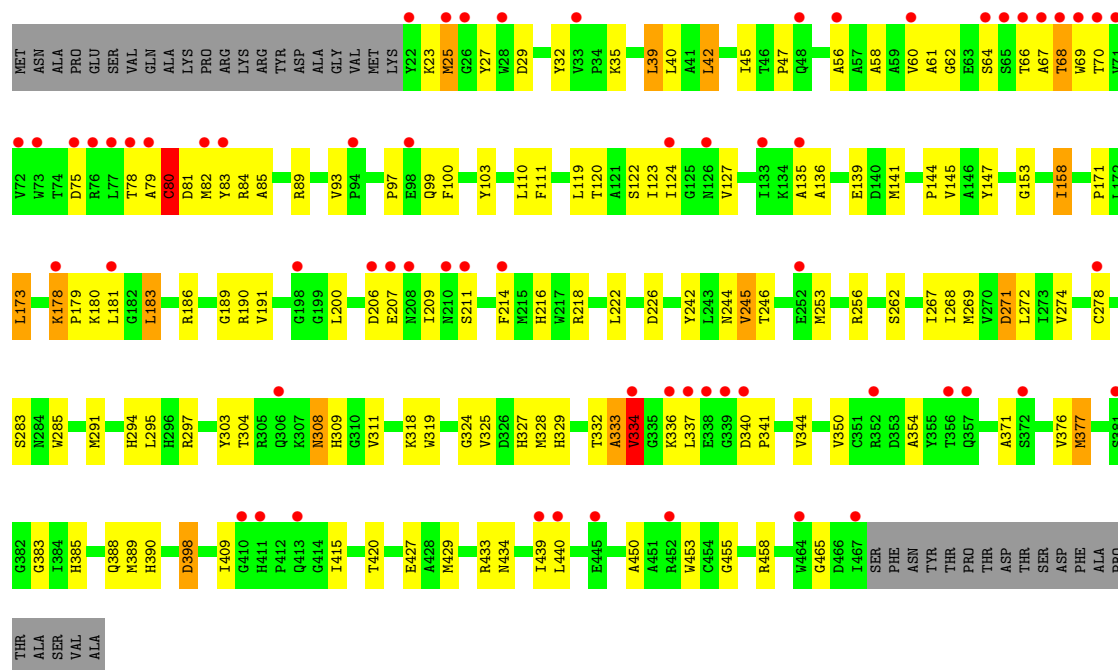


• Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)

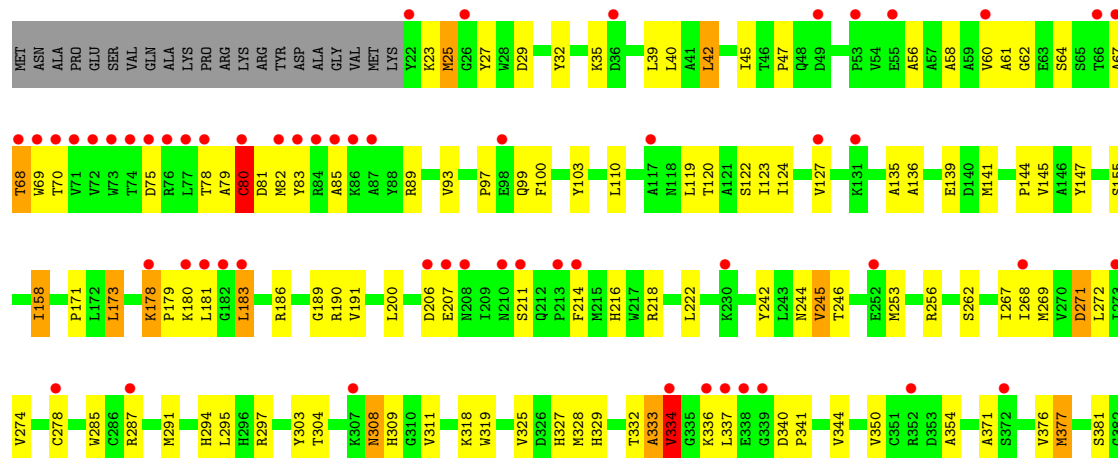


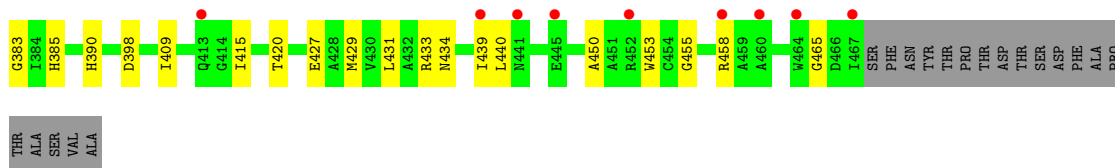


● Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)



● Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)





• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.00Å 112.00Å 402.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.0 (15.00-2.70) 86.3 (15.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.64Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.266 , 0.322 0.280 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.1	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	0.89	EDS
Total number of atoms	18144	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: PO4

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	0.40	0/3552	0.88	3/4816 (0.1%)
1	C	0.41	0/3552	0.87	4/4816 (0.1%)
1	E	0.40	0/3552	0.88	5/4816 (0.1%)
1	G	0.41	0/3552	0.88	3/4816 (0.1%)
2	I	0.42	0/1084	0.89	4/1474 (0.3%)
2	J	0.40	0/1084	0.89	2/1474 (0.1%)
2	K	0.40	0/1084	0.89	2/1474 (0.1%)
2	L	0.40	0/1084	0.89	2/1474 (0.1%)
All	All	0.40	0/18544	0.88	25/25160 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	ALA	N-CA-C	-6.71	104.11	112.90
1	A	354	ALA	N-CA-C	-6.68	104.15	112.90
2	L	48	TRP	N-CA-C	-6.61	102.00	110.53
2	K	48	TRP	N-CA-C	-6.58	102.32	110.41
1	G	354	ALA	N-CA-C	-6.58	104.29	112.90
1	E	354	ALA	N-CA-C	-6.57	104.30	112.90
2	J	48	TRP	N-CA-C	-6.48	102.17	110.53
2	I	48	TRP	N-CA-C	-6.42	102.25	110.53
2	I	45	ASN	N-CA-C	-6.28	100.85	109.71
2	K	45	ASN	N-CA-C	-6.24	100.92	109.71
2	J	45	ASN	N-CA-C	-6.21	100.96	109.71
2	L	45	ASN	N-CA-C	-6.12	101.08	109.71
1	C	178	LYS	N-CA-C	5.90	121.71	113.57
1	A	178	LYS	N-CA-C	5.89	121.70	113.57
1	E	178	LYS	N-CA-C	5.88	121.69	113.57
1	G	178	LYS	N-CA-C	5.80	121.58	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	ASP	N-CA-C	-5.31	105.57	111.36
2	I	106	GLU	CA-C-N	5.14	124.86	119.82
2	I	106	GLU	C-N-CA	5.14	124.86	119.82
1	C	207	GLU	N-CA-C	5.10	121.67	110.80
1	E	158	ILE	N-CA-C	5.09	115.53	110.23
1	A	158	ILE	N-CA-C	5.08	115.52	110.23
1	E	398	ASP	N-CA-C	5.08	117.93	111.69
1	C	226	ASP	N-CA-C	-5.02	105.89	111.36
1	G	158	ILE	N-CA-C	5.01	115.44	110.23

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	3470	0	3402	101	0
1	C	3470	0	3402	97	0
1	E	3470	0	3402	97	0
1	G	3470	0	3402	93	0
2	I	1056	0	1007	40	0
2	J	1056	0	1007	42	0
2	K	1056	0	1007	42	0
2	L	1056	0	1007	45	0
3	A	10	0	0	0	0
3	C	10	0	0	0	0
3	E	10	0	0	0	0
3	G	10	0	0	1	0
All	All	18144	0	17636	516	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 14.

All (516) 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:429:MET:HE2	1:C:439:ILE:HG23	1.56	0.85
1:E:429:MET:HE2	1:E:439:ILE:HG23	1.58	0.84
1:A:429:MET:HE2	1:A:439:ILE:HG23	1.59	0.83
1:G:429:MET:HE2	1:G:439:ILE:HG23	1.59	0.82
1:A:420:THR:HG23	2:I:10:PHE:HE2	1.48	0.79
1:G:433:ARG:HH21	1:G:434:ASN:HD21	1.31	0.78
1:C:420:THR:HG23	2:J:10:PHE:HE2	1.50	0.77
1:C:433:ARG:HH21	1:C:434:ASN:HD21	1.32	0.77
1:E:433:ARG:HH21	1:E:434:ASN:HD21	1.29	0.77
2:J:38:THR:HG22	2:J:40:ASP:H	1.51	0.76
1:A:433:ARG:HH21	1:A:434:ASN:HD21	1.30	0.76
2:K:38:THR:HG22	2:K:40:ASP:H	1.52	0.75
1:A:245:VAL:HG21	1:A:268:ILE:HD11	1.69	0.74
1:E:420:THR:HG23	2:K:10:PHE:HE2	1.51	0.74
2:I:38:THR:HG22	2:I:40:ASP:H	1.52	0.74
2:J:112:VAL:HB	2:J:124:SER:HB2	1.70	0.74
2:K:112:VAL:HB	2:K:124:SER:HB2	1.69	0.74
2:L:38:THR:HG22	2:L:40:ASP:H	1.51	0.73
1:C:245:VAL:HG21	1:C:268:ILE:HD11	1.71	0.73
2:K:104:ALA:O	2:K:107:PRO:HD3	1.89	0.73
1:G:245:VAL:HG21	1:G:268:ILE:HD11	1.69	0.72
1:G:420:THR:HG23	2:L:10:PHE:HE2	1.54	0.72
2:L:83:THR:HG22	2:L:95:VAL:HG22	1.70	0.72
1:G:158:ILE:HG12	1:G:377:MET:HG2	1.72	0.72
1:C:158:ILE:HG12	1:C:377:MET:HG2	1.70	0.72
2:L:55:MET:HG3	2:L:64:ILE:HG12	1.72	0.72
2:L:104:ALA:O	2:L:107:PRO:HD3	1.89	0.72
2:J:104:ALA:O	2:J:107:PRO:HD3	1.90	0.72
2:I:112:VAL:HB	2:I:124:SER:HB2	1.72	0.71
1:E:245:VAL:HG21	1:E:268:ILE:HD11	1.71	0.71
2:J:83:THR:HG22	2:J:95:VAL:HG22	1.72	0.71
2:I:55:MET:HG3	2:I:64:ILE:HG12	1.71	0.71
1:A:158:ILE:HG12	1:A:377:MET:HG2	1.73	0.71
2:K:83:THR:HG22	2:K:95:VAL:HG22	1.73	0.70
2:K:25:TYR:O	2:K:29:GLN:HG2	1.91	0.70
2:L:112:VAL:HB	2:L:124:SER:HB2	1.72	0.70
2:I:83:THR:HG22	2:I:95:VAL:HG22	1.71	0.70
1:G:332:THR:HG21	1:G:336:LYS:HB3	1.74	0.70
1:A:297:ARG:HG2	1:A:329:HIS:HB2	1.74	0.69
2:I:104:ALA:O	2:I:107:PRO:HD3	1.91	0.69
1:G:297:ARG:HG2	1:G:329:HIS:HB2	1.74	0.69
2:I:25:TYR:O	2:I:29:GLN:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:THR:HG21	1:E:336:LYS:HB3	1.74	0.69
2:K:55:MET:HG3	2:K:64:ILE:HG12	1.75	0.69
1:C:297:ARG:HG2	1:C:329:HIS:HB2	1.75	0.69
1:A:332:THR:HG21	1:A:336:LYS:HB3	1.74	0.68
1:C:332:THR:HG21	1:C:336:LYS:HB3	1.75	0.68
2:J:47:TYR:HA	1:E:190:ARG:NH2	2.08	0.68
1:E:158:ILE:HG12	1:E:377:MET:HG2	1.73	0.68
1:E:297:ARG:HG2	1:E:329:HIS:HB2	1.76	0.68
2:J:55:MET:HG3	2:J:64:ILE:HG12	1.75	0.68
2:J:25:TYR:O	2:J:29:GLN:HG2	1.93	0.67
1:E:179:PRO:HB3	1:E:183:LEU:HD13	1.77	0.67
1:A:179:PRO:HB3	1:A:183:LEU:HD13	1.76	0.67
2:L:25:TYR:O	2:L:29:GLN:HG2	1.94	0.67
1:G:179:PRO:HB3	1:G:183:LEU:HD13	1.77	0.66
1:A:183:LEU:HA	2:L:90:THR:HB	1.78	0.66
1:G:62:GLY:O	1:G:67:ALA:HB3	1.96	0.66
1:E:62:GLY:O	1:E:67:ALA:HB3	1.96	0.65
1:A:62:GLY:O	1:A:67:ALA:HB3	1.96	0.65
1:E:242:TYR:HB3	1:E:269:MET:HB2	1.78	0.65
1:C:179:PRO:HB3	1:C:183:LEU:HD13	1.77	0.64
1:C:242:TYR:HB3	1:C:269:MET:HB2	1.79	0.64
1:C:62:GLY:O	1:C:67:ALA:HB3	1.98	0.64
1:A:420:THR:HG23	2:I:10:PHE:CE2	2.32	0.63
1:A:242:TYR:HB3	1:A:269:MET:HB2	1.81	0.63
1:A:180:LYS:HG2	1:A:181:LEU:H	1.64	0.63
1:C:328:MET:HE3	1:C:376:VAL:HG11	1.81	0.62
1:E:328:MET:HE3	1:E:376:VAL:HG11	1.80	0.62
2:K:50:MET:HE3	1:G:190:ARG:HD3	1.82	0.62
1:C:334:VAL:HB	1:C:341:PRO:HG3	1.82	0.62
1:A:328:MET:HE3	1:A:376:VAL:HG11	1.82	0.61
1:G:242:TYR:HB3	1:G:269:MET:HB2	1.82	0.61
1:E:180:LYS:HG2	1:E:181:LEU:H	1.66	0.61
1:G:274:VAL:HG12	1:G:278:CYS:CB	2.30	0.61
1:E:334:VAL:HB	1:E:341:PRO:HG3	1.83	0.61
2:K:90:THR:HB	1:G:183:LEU:HA	1.83	0.60
1:G:35:LYS:NZ	1:G:82:MET:HE1	2.15	0.60
1:A:123:ILE:HG13	1:A:141:MET:HE1	1.83	0.60
1:A:274:VAL:HG12	1:A:278:CYS:CB	2.30	0.60
1:A:35:LYS:NZ	1:A:82:MET:HE1	2.16	0.60
1:G:334:VAL:HB	1:G:341:PRO:HG3	1.83	0.60
1:G:180:LYS:HG2	1:G:181:LEU:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:LYS:NZ	1:E:82:MET:HE1	2.16	0.60
1:C:35:LYS:NZ	1:C:82:MET:HE1	2.17	0.60
1:C:180:LYS:HG2	1:C:181:LEU:H	1.67	0.59
1:C:274:VAL:HG12	1:C:278:CYS:CB	2.31	0.59
1:E:123:ILE:HG13	1:E:141:MET:HE1	1.84	0.59
2:L:44:ARG:HH11	2:L:44:ARG:HA	1.67	0.59
1:C:136:ALA:O	1:C:309:HIS:HA	2.03	0.59
1:A:334:VAL:HB	1:A:341:PRO:HG3	1.84	0.59
1:A:145:VAL:HG13	1:A:371:ALA:HB2	1.85	0.59
1:E:274:VAL:HG12	1:E:278:CYS:CB	2.32	0.59
1:A:190:ARG:HD3	2:L:50:MET:HE3	1.84	0.59
1:E:61:ALA:HB1	1:E:85:ALA:O	2.03	0.59
2:J:44:ARG:HH11	2:J:44:ARG:HA	1.69	0.58
1:G:61:ALA:HB1	1:G:85:ALA:O	2.03	0.58
1:A:433:ARG:HG3	1:A:439:ILE:HD11	1.86	0.58
1:C:61:ALA:HB1	1:C:85:ALA:O	2.04	0.58
1:C:333:ALA:HB2	1:C:344:VAL:HG11	1.86	0.58
2:K:44:ARG:HA	2:K:44:ARG:HH11	1.66	0.58
2:I:50:MET:HE3	1:C:190:ARG:HD3	1.85	0.58
1:E:433:ARG:HG3	1:E:439:ILE:HD11	1.85	0.58
1:G:245:VAL:HG22	1:G:256:ARG:HB2	1.84	0.58
1:E:68:THR:HG23	1:E:70:THR:O	2.04	0.57
1:C:420:THR:HG23	2:J:10:PHE:CE2	2.34	0.57
1:C:433:ARG:HG3	1:C:439:ILE:HD11	1.85	0.57
1:A:433:ARG:HH21	1:A:434:ASN:ND2	2.00	0.57
2:K:15:THR:H	2:K:18:GLN:HE21	1.52	0.57
1:A:189:GLY:HA3	2:L:47:TYR:OH	2.05	0.57
1:A:333:ALA:HB2	1:A:344:VAL:HG11	1.87	0.57
2:J:90:THR:HB	1:E:183:LEU:HA	1.87	0.57
1:G:123:ILE:HG13	1:G:141:MET:HE1	1.86	0.57
1:A:61:ALA:HB1	1:A:85:ALA:O	2.04	0.57
2:I:15:THR:H	2:I:18:GLN:HE21	1.52	0.57
1:A:68:THR:HG23	1:A:70:THR:O	2.05	0.57
1:A:433:ARG:NH2	1:A:434:ASN:HD21	2.02	0.57
1:C:68:THR:HG23	1:C:70:THR:O	2.05	0.57
2:I:44:ARG:HA	2:I:44:ARG:HH11	1.68	0.57
1:C:145:VAL:HG13	1:C:371:ALA:HB2	1.85	0.57
2:J:15:THR:H	2:J:18:GLN:HE21	1.53	0.57
1:E:245:VAL:HG22	1:E:256:ARG:HB2	1.87	0.57
1:G:328:MET:HE3	1:G:376:VAL:HG11	1.85	0.57
1:E:23:LYS:HA	1:E:58:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ARG:HH21	1:E:434:ASN:ND2	2.00	0.56
1:G:336:LYS:HG3	1:G:383:GLY:H	1.70	0.56
1:G:136:ALA:O	1:G:309:HIS:HA	2.05	0.56
1:C:336:LYS:HG3	1:C:383:GLY:H	1.70	0.56
1:E:136:ALA:O	1:E:309:HIS:HA	2.05	0.56
1:E:145:VAL:HG13	1:E:371:ALA:HB2	1.86	0.56
1:E:179:PRO:HG2	1:E:191:VAL:HG21	1.88	0.56
1:G:274:VAL:HG12	1:G:278:CYS:HB2	1.88	0.56
1:G:433:ARG:HG3	1:G:439:ILE:HD11	1.86	0.56
2:L:38:THR:HG1	2:L:48:TRP:CG	2.23	0.56
1:G:68:THR:HG23	1:G:70:THR:O	2.05	0.56
1:G:145:VAL:HG13	1:G:371:ALA:HB2	1.87	0.56
1:A:23:LYS:HA	1:A:58:ALA:HB1	1.86	0.56
1:E:420:THR:HG23	2:K:10:PHE:CE2	2.36	0.56
1:E:433:ARG:NH2	1:E:434:ASN:HD21	2.02	0.56
1:A:336:LYS:HG3	1:A:383:GLY:H	1.70	0.56
2:I:90:THR:HB	1:C:183:LEU:HA	1.88	0.56
1:G:23:LYS:HA	1:G:58:ALA:HB1	1.87	0.56
1:C:123:ILE:HG13	1:C:141:MET:HE1	1.87	0.56
1:A:337:LEU:H	1:A:337:LEU:HD22	1.71	0.55
1:G:433:ARG:NH2	1:G:434:ASN:HD21	2.02	0.55
1:E:336:LYS:HG3	1:E:383:GLY:H	1.70	0.55
1:C:433:ARG:NH2	1:C:434:ASN:HD21	2.04	0.55
2:J:82:VAL:HG23	2:J:98:PHE:CE1	2.42	0.55
1:G:333:ALA:HB2	1:G:344:VAL:HG11	1.88	0.55
1:C:93:VAL:HG23	1:C:100:PHE:HA	1.88	0.55
1:A:216:HIS:HD2	1:A:218:ARG:HB2	1.72	0.55
2:I:82:VAL:HG23	2:I:98:PHE:CE1	2.42	0.55
2:I:82:VAL:HG23	2:I:98:PHE:HE1	1.72	0.55
1:C:245:VAL:HG22	1:C:256:ARG:HB2	1.87	0.55
1:A:93:VAL:HG23	1:A:100:PHE:HA	1.88	0.55
1:A:245:VAL:HG22	1:A:256:ARG:HB2	1.89	0.55
2:I:47:TYR:HA	1:C:190:ARG:NH2	2.22	0.55
1:C:23:LYS:HA	1:C:58:ALA:HB1	1.87	0.55
1:E:253:MET:HE1	1:E:274:VAL:HG11	1.89	0.54
1:G:337:LEU:HD22	1:G:337:LEU:H	1.72	0.54
1:C:433:ARG:HH21	1:C:434:ASN:ND2	2.02	0.54
2:K:114:GLN:HB3	2:K:122:ARG:HB3	1.89	0.54
1:A:274:VAL:HG12	1:A:278:CYS:HB2	1.88	0.54
1:E:304:THR:HG22	1:E:311:VAL:O	2.08	0.54
1:A:136:ALA:O	1:A:309:HIS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:82:VAL:HG23	2:J:98:PHE:HE1	1.71	0.54
1:A:304:THR:HG22	1:A:311:VAL:O	2.08	0.54
2:K:82:VAL:HG23	2:K:98:PHE:HE1	1.73	0.54
1:G:216:HIS:HD2	1:G:218:ARG:HB2	1.72	0.54
1:C:179:PRO:HG2	1:C:191:VAL:HG21	1.90	0.54
1:E:216:HIS:HD2	1:E:218:ARG:HB2	1.72	0.54
1:C:337:LEU:HD22	1:C:337:LEU:H	1.73	0.53
1:G:433:ARG:HH21	1:G:434:ASN:ND2	2.01	0.53
2:L:82:VAL:HG23	2:L:98:PHE:HE1	1.73	0.53
2:K:82:VAL:HG23	2:K:98:PHE:CE1	2.43	0.53
1:A:253:MET:HE1	1:A:274:VAL:HG11	1.89	0.53
1:G:304:THR:HG22	1:G:311:VAL:O	2.08	0.53
1:E:274:VAL:HG12	1:E:278:CYS:HB2	1.89	0.53
1:E:337:LEU:HD22	1:E:337:LEU:H	1.72	0.53
1:G:93:VAL:HG23	1:G:100:PHE:HA	1.89	0.53
2:J:116:GLU:HB3	2:J:117:PRO:HD2	1.91	0.53
1:G:318:LYS:HG2	1:G:350:VAL:HG13	1.90	0.53
1:E:294:HIS:HA	1:E:327:HIS:HB2	1.91	0.53
1:G:420:THR:HG23	2:L:10:PHE:CE2	2.38	0.53
2:K:47:TYR:HA	1:G:190:ARG:NH2	2.23	0.53
2:I:38:THR:HG1	2:I:48:TRP:CG	2.26	0.53
1:E:93:VAL:HG23	1:E:100:PHE:HA	1.89	0.53
2:L:114:GLN:HB3	2:L:122:ARG:HB3	1.91	0.53
1:C:253:MET:HE1	1:C:274:VAL:HG11	1.90	0.53
1:C:274:VAL:HG12	1:C:278:CYS:HB2	1.89	0.53
2:K:1:MET:SD	2:K:107:PRO:HD2	2.48	0.53
2:L:11:LEU:HB3	2:L:12:PRO:HD2	1.91	0.53
1:C:304:THR:HG22	1:C:311:VAL:O	2.09	0.52
1:A:190:ARG:NH2	2:L:47:TYR:HA	2.24	0.52
2:L:15:THR:H	2:L:18:GLN:HE21	1.56	0.52
1:C:216:HIS:HD2	1:C:218:ARG:HB2	1.74	0.52
1:E:333:ALA:HB2	1:E:344:VAL:HG11	1.90	0.52
2:I:1:MET:SD	2:I:107:PRO:HD2	2.49	0.52
2:I:114:GLN:HB3	2:I:122:ARG:HB3	1.92	0.52
2:J:114:GLN:HB3	2:J:122:ARG:HB3	1.92	0.52
2:L:82:VAL:HG23	2:L:98:PHE:CE1	2.43	0.52
1:A:318:LYS:HG2	1:A:350:VAL:HG13	1.92	0.52
1:C:83:TYR:HA	1:C:110:LEU:HD21	1.92	0.52
1:G:179:PRO:HG2	1:G:191:VAL:HG21	1.91	0.52
1:G:381:SER:HB3	3:G:507:PO4:O3	2.10	0.52
1:C:294:HIS:HA	1:C:327:HIS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:TRP:H	1:E:69:TRP:CD1	2.28	0.52
2:K:104:ALA:HB1	2:K:107:PRO:HG3	1.92	0.52
1:G:69:TRP:H	1:G:69:TRP:CD1	2.28	0.52
1:G:294:HIS:HA	1:G:327:HIS:HB2	1.92	0.51
1:A:179:PRO:HG2	1:A:191:VAL:HG21	1.91	0.51
2:K:11:LEU:HB3	2:K:12:PRO:HD2	1.93	0.51
1:A:294:HIS:HA	1:A:327:HIS:HB2	1.93	0.51
2:J:1:MET:SD	2:J:107:PRO:HD2	2.50	0.51
2:J:11:LEU:HB3	2:J:12:PRO:HD2	1.92	0.51
2:J:104:ALA:HB1	2:J:107:PRO:HG3	1.93	0.51
1:C:262:SER:HA	2:K:117:PRO:HB3	1.92	0.51
1:E:178:LYS:HB3	1:E:409:ILE:HG21	1.93	0.51
1:A:69:TRP:CD1	1:A:69:TRP:H	2.28	0.51
1:G:64:SER:HB2	1:G:122:SER:O	2.11	0.51
2:J:47:TYR:OH	1:E:189:GLY:HA3	2.10	0.51
2:L:104:ALA:HB1	2:L:107:PRO:HG3	1.92	0.51
2:K:17:GLU:O	2:K:21:LYS:HG3	2.11	0.50
1:C:69:TRP:CD1	1:C:69:TRP:H	2.28	0.50
1:C:295:LEU:HB2	1:C:325:VAL:CG1	2.42	0.50
1:E:295:LEU:HB2	1:E:325:VAL:CG1	2.41	0.50
2:I:11:LEU:HB3	2:I:12:PRO:HD2	1.94	0.50
2:I:47:TYR:OH	1:C:189:GLY:HA3	2.12	0.50
2:J:38:THR:HG1	2:J:48:TRP:CG	2.29	0.50
2:I:104:ALA:HB1	2:I:107:PRO:HG3	1.94	0.50
1:E:318:LYS:HG2	1:E:350:VAL:HG13	1.92	0.50
1:G:253:MET:HE1	1:G:274:VAL:HG11	1.93	0.50
1:E:64:SER:HB2	1:E:122:SER:O	2.11	0.50
2:L:1:MET:SD	2:L:107:PRO:HD2	2.51	0.50
2:L:116:GLU:HB3	2:L:117:PRO:HD2	1.94	0.50
2:I:116:GLU:HB3	2:I:117:PRO:HD2	1.93	0.49
1:A:183:LEU:HG	2:L:90:THR:HG21	1.95	0.49
2:K:47:TYR:OH	1:G:189:GLY:HA3	2.12	0.49
1:E:427:GLU:HG3	2:K:10:PHE:HB2	1.94	0.49
1:C:318:LYS:HG2	1:C:350:VAL:HG13	1.93	0.49
1:G:178:LYS:HB3	1:G:409:ILE:HG21	1.94	0.49
1:G:333:ALA:O	1:G:334:VAL:HG12	2.13	0.49
2:L:4:THR:O	2:L:4:THR:HG22	2.13	0.49
2:J:50:MET:HE3	1:E:190:ARG:HD3	1.94	0.49
1:C:35:LYS:HZ2	1:C:82:MET:HE1	1.78	0.49
1:E:35:LYS:HZ2	1:E:82:MET:HE1	1.78	0.49
2:K:4:THR:HG22	2:K:4:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:GLU:O	2:L:21:LYS:HG3	2.13	0.49
1:A:333:ALA:O	1:A:334:VAL:HG12	2.13	0.49
2:J:104:ALA:O	2:J:105:ASP:C	2.55	0.49
1:G:271:ASP:O	1:G:274:VAL:HG23	2.13	0.49
1:G:295:LEU:HB2	1:G:325:VAL:CG1	2.43	0.49
1:A:29:ASP:HB3	1:A:32:TYR:HB2	1.95	0.48
1:G:27:TYR:CZ	1:G:67:ALA:HB2	2.48	0.48
1:A:178:LYS:HB3	1:A:409:ILE:HG21	1.94	0.48
2:K:116:GLU:HB3	2:K:117:PRO:HD2	1.94	0.48
1:C:271:ASP:O	1:C:274:VAL:HG23	2.13	0.48
1:E:45:ILE:HG22	1:E:47:PRO:HD3	1.95	0.48
2:K:38:THR:HG1	2:K:48:TRP:CG	2.31	0.48
2:I:4:THR:O	2:I:4:THR:HG22	2.14	0.48
1:C:89:ARG:HB2	1:C:103:TYR:HB2	1.96	0.48
2:J:112:VAL:O	2:J:123:TYR:HA	2.12	0.48
1:G:40:LEU:O	1:G:141:MET:HA	2.12	0.48
1:G:89:ARG:HB2	1:G:103:TYR:HB2	1.96	0.48
1:G:120:THR:HG22	1:G:319:TRP:CH2	2.48	0.48
2:K:104:ALA:O	2:K:105:ASP:C	2.56	0.48
1:A:64:SER:HB2	1:A:122:SER:O	2.13	0.48
1:A:271:ASP:O	1:A:274:VAL:HG23	2.13	0.48
1:E:40:LEU:O	1:E:141:MET:HA	2.14	0.48
2:I:112:VAL:O	2:I:123:TYR:HA	2.13	0.48
1:C:64:SER:HB2	1:C:122:SER:O	2.13	0.48
1:E:333:ALA:O	1:E:334:VAL:HG12	2.13	0.48
2:I:117:PRO:HB3	1:G:262:SER:HA	1.95	0.48
1:C:27:TYR:CZ	1:C:67:ALA:HB2	2.49	0.48
1:C:178:LYS:HB3	1:C:409:ILE:HG21	1.96	0.48
1:E:295:LEU:HB2	1:E:325:VAL:HG11	1.96	0.48
1:C:245:VAL:HG13	1:C:253:MET:HG3	1.96	0.47
1:A:83:TYR:HA	1:A:110:LEU:HD21	1.95	0.47
2:I:17:GLU:O	2:I:21:LYS:HG3	2.14	0.47
2:J:4:THR:HG22	2:J:4:THR:O	2.14	0.47
2:J:17:GLU:O	2:J:21:LYS:HG3	2.14	0.47
1:E:83:TYR:HA	1:E:110:LEU:HD21	1.95	0.47
1:G:244:ASN:ND2	1:G:246:THR:H	2.12	0.47
1:A:124:ILE:O	1:A:127:VAL:HG22	2.14	0.47
1:C:144:PRO:HG2	1:C:147:TYR:HB2	1.97	0.47
2:I:104:ALA:O	2:I:105:ASP:C	2.56	0.47
1:C:295:LEU:HB2	1:C:325:VAL:HG11	1.95	0.47
1:E:262:SER:HA	2:L:117:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:ALA:O	2:L:105:ASP:C	2.56	0.47
1:C:124:ILE:O	1:C:127:VAL:HG22	2.14	0.47
2:L:112:VAL:O	2:L:123:TYR:HA	2.14	0.47
1:A:27:TYR:CZ	1:A:67:ALA:HB2	2.49	0.47
1:A:89:ARG:HB2	1:A:103:TYR:HB2	1.96	0.47
1:C:29:ASP:HB3	1:C:32:TYR:HB2	1.97	0.47
1:E:27:TYR:CZ	1:E:67:ALA:HB2	2.50	0.47
1:A:120:THR:HG22	1:A:319:TRP:CZ3	2.50	0.47
1:A:295:LEU:HB2	1:A:325:VAL:CG1	2.44	0.47
1:C:120:THR:HG22	1:C:319:TRP:CH2	2.49	0.47
1:E:89:ARG:HB2	1:E:103:TYR:HB2	1.97	0.47
1:E:433:ARG:HG3	1:E:439:ILE:CD1	2.45	0.47
1:C:333:ALA:O	1:C:334:VAL:HG12	2.14	0.47
2:J:46:THR:HG21	1:E:186:ARG:HG3	1.96	0.47
1:E:124:ILE:O	1:E:127:VAL:HG22	2.14	0.47
1:E:144:PRO:HG2	1:E:147:TYR:HB2	1.96	0.47
1:G:35:LYS:HZ2	1:G:82:MET:HE1	1.80	0.47
1:G:120:THR:HG22	1:G:319:TRP:CZ3	2.50	0.47
2:I:65:LEU:HA	2:I:68:ILE:HD12	1.97	0.47
1:C:171:PRO:HA	1:C:398:ASP:O	2.15	0.47
1:A:144:PRO:HG2	1:A:147:TYR:HB2	1.96	0.46
2:I:113:ARG:HB3	2:I:121:LEU:HD22	1.96	0.46
1:C:244:ASN:ND2	1:C:246:THR:H	2.13	0.46
1:E:120:THR:HG22	1:E:319:TRP:CH2	2.50	0.46
1:A:120:THR:HG22	1:A:319:TRP:CH2	2.51	0.46
1:C:390:HIS:CD2	1:C:390:HIS:H	2.34	0.46
1:C:450:ALA:HA	1:C:453:TRP:NE1	2.31	0.46
1:E:271:ASP:O	1:E:274:VAL:HG23	2.15	0.46
1:A:431:LEU:HD12	2:I:22:GLN:OE1	2.15	0.46
1:E:78:THR:C	1:E:80:CYS:H	2.24	0.46
1:E:120:THR:HG22	1:E:319:TRP:CZ3	2.50	0.46
1:C:433:ARG:HG3	1:C:439:ILE:CD1	2.45	0.46
1:G:124:ILE:O	1:G:127:VAL:HG22	2.15	0.46
1:A:80:CYS:O	1:A:82:MET:N	2.49	0.46
1:E:415:ILE:HD12	1:E:415:ILE:H	1.81	0.46
1:A:245:VAL:HG13	1:A:253:MET:HG3	1.97	0.46
1:A:433:ARG:HG3	1:A:439:ILE:CD1	2.46	0.46
1:C:78:THR:C	1:C:80:CYS:H	2.24	0.46
1:E:245:VAL:HG13	1:E:253:MET:HG3	1.98	0.46
1:G:390:HIS:CD2	1:G:390:HIS:H	2.33	0.46
1:A:262:SER:HA	2:J:117:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ASP:HB3	1:E:32:TYR:HB2	1.97	0.46
2:K:112:VAL:O	2:K:123:TYR:HA	2.16	0.46
1:G:450:ALA:HA	1:G:453:TRP:NE1	2.31	0.46
1:A:45:ILE:HG22	1:A:47:PRO:HD3	1.97	0.46
1:G:29:ASP:HB3	1:G:32:TYR:HB2	1.97	0.45
1:G:78:THR:C	1:G:80:CYS:H	2.24	0.45
1:A:78:THR:C	1:A:80:CYS:H	2.24	0.45
1:A:244:ASN:ND2	1:A:246:THR:H	2.15	0.45
2:K:65:LEU:HA	2:K:68:ILE:HD12	1.99	0.45
1:A:171:PRO:HA	1:A:398:ASP:O	2.15	0.45
1:G:42:LEU:HD13	1:G:139:GLU:HB2	1.98	0.45
1:G:69:TRP:H	1:G:69:TRP:HD1	1.64	0.45
1:G:285:TRP:CZ3	1:G:291:MET:HG3	2.51	0.45
1:E:450:ALA:HA	1:E:453:TRP:NE1	2.31	0.45
1:E:171:PRO:HA	1:E:398:ASP:O	2.17	0.45
1:E:244:ASN:ND2	1:E:246:THR:H	2.15	0.45
2:K:46:THR:HG21	1:G:186:ARG:HG3	1.97	0.45
1:A:390:HIS:H	1:A:390:HIS:CD2	2.35	0.45
1:A:450:ALA:HA	1:A:453:TRP:NE1	2.31	0.45
1:E:455:GLY:O	1:E:458:ARG:HB3	2.16	0.45
1:G:171:PRO:HA	1:G:398:ASP:O	2.16	0.45
2:I:109:PHE:HD1	2:I:109:PHE:H	1.64	0.45
1:C:120:THR:HG22	1:C:319:TRP:CZ3	2.51	0.45
1:E:69:TRP:H	1:E:69:TRP:HD1	1.65	0.45
1:E:135:ALA:HB1	1:E:308:ASN:O	2.17	0.45
1:A:40:LEU:O	1:A:141:MET:HA	2.16	0.45
1:A:415:ILE:HD12	1:A:415:ILE:H	1.81	0.45
1:C:40:LEU:O	1:C:141:MET:HA	2.16	0.45
2:L:65:LEU:HA	2:L:68:ILE:HD12	1.97	0.45
1:C:80:CYS:O	1:C:82:MET:N	2.50	0.45
1:E:390:HIS:CD2	1:E:390:HIS:H	2.35	0.45
1:G:144:PRO:HG2	1:G:147:TYR:HB2	1.98	0.45
1:A:79:ALA:C	1:A:80:CYS:SG	3.00	0.45
1:C:45:ILE:HG22	1:C:47:PRO:HD3	1.98	0.45
1:C:455:GLY:O	1:C:458:ARG:HB3	2.17	0.44
1:E:385:HIS:HE1	1:E:465:GLY:O	2.00	0.44
1:G:83:TYR:HA	1:G:110:LEU:HD21	1.97	0.44
1:G:135:ALA:HB1	1:G:308:ASN:O	2.17	0.44
2:J:109:PHE:HD1	2:J:109:PHE:H	1.66	0.44
1:E:295:LEU:CB	1:E:325:VAL:HG11	2.47	0.44
1:G:295:LEU:HB2	1:G:325:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HB2	1:A:325:VAL:HG11	1.99	0.44
2:J:113:ARG:HB3	2:J:121:LEU:HD22	1.98	0.44
1:E:80:CYS:O	1:E:82:MET:N	2.50	0.44
2:L:109:PHE:H	2:L:109:PHE:HD1	1.65	0.44
1:C:173:LEU:HD13	1:C:200:LEU:HD23	1.99	0.44
2:J:37:TYR:HA	2:J:79:TYR:O	2.18	0.44
1:E:336:LYS:HG3	1:E:383:GLY:N	2.33	0.44
1:G:79:ALA:C	1:G:80:CYS:SG	3.00	0.44
1:G:80:CYS:O	1:G:82:MET:N	2.51	0.44
1:G:245:VAL:HG13	1:G:253:MET:HG3	1.99	0.44
1:A:455:GLY:O	1:A:458:ARG:HB3	2.17	0.44
1:C:415:ILE:HD12	1:C:415:ILE:H	1.83	0.44
1:C:431:LEU:HD12	2:J:22:GLN:OE1	2.18	0.44
1:E:303:TYR:CD1	1:E:304:THR:HG23	2.53	0.44
1:G:45:ILE:HG22	1:G:47:PRO:HD3	2.00	0.44
1:G:385:HIS:HE1	1:G:465:GLY:O	1.99	0.44
1:C:427:GLU:HG3	2:J:10:PHE:HB2	2.00	0.44
2:J:65:LEU:HA	2:J:68:ILE:HD12	1.98	0.44
1:C:340:ASP:O	1:C:344:VAL:HG23	2.18	0.44
1:G:427:GLU:HG3	2:L:10:PHE:HB2	2.00	0.44
1:G:455:GLY:O	1:G:458:ARG:HB3	2.17	0.44
1:E:439:ILE:H	1:E:439:ILE:HG13	1.56	0.44
1:G:340:ASP:O	1:G:344:VAL:HG23	2.18	0.44
1:A:340:ASP:O	1:A:344:VAL:HG23	2.18	0.43
1:C:295:LEU:CB	1:C:325:VAL:HG11	2.48	0.43
1:C:385:HIS:HE1	1:C:465:GLY:O	2.01	0.43
1:A:283:SER:OG	1:A:324:GLY:HA3	2.18	0.43
1:A:385:HIS:HE1	1:A:465:GLY:O	2.00	0.43
1:G:336:LYS:HG3	1:G:383:GLY:N	2.33	0.43
1:C:180:LYS:HG3	1:C:206:ASP:HB3	2.00	0.43
2:K:37:TYR:HA	2:K:79:TYR:O	2.19	0.43
1:G:433:ARG:HG3	1:G:439:ILE:CD1	2.47	0.43
1:C:283:SER:OG	1:C:324:GLY:HA3	2.18	0.43
1:C:336:LYS:HG3	1:C:383:GLY:N	2.33	0.43
2:I:37:TYR:HA	2:I:79:TYR:O	2.18	0.43
1:C:135:ALA:HB1	1:C:308:ASN:O	2.19	0.43
2:K:109:PHE:HD1	2:K:109:PHE:H	1.64	0.43
1:G:415:ILE:HD12	1:G:415:ILE:H	1.84	0.43
1:A:69:TRP:H	1:A:69:TRP:HD1	1.66	0.43
2:I:45:ASN:ND2	2:J:113:ARG:HH22	2.16	0.43
1:E:42:LEU:HD13	1:E:139:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:TYR:HA	2:L:79:TYR:O	2.18	0.43
2:I:113:ARG:HH22	2:L:45:ASN:ND2	2.17	0.43
1:G:295:LEU:CB	1:G:325:VAL:HG11	2.49	0.43
1:A:135:ALA:HB1	1:A:308:ASN:O	2.19	0.43
1:A:253:MET:HE1	1:A:274:VAL:CG1	2.49	0.43
2:K:113:ARG:HB3	2:K:121:LEU:HD22	2.01	0.43
1:A:144:PRO:HG2	1:A:147:TYR:CB	2.49	0.43
1:C:79:ALA:C	1:C:80:CYS:SG	3.01	0.43
2:K:68:ILE:HD13	2:K:98:PHE:CE1	2.53	0.43
2:K:90:THR:HG21	1:G:183:LEU:HG	2.01	0.43
1:C:69:TRP:H	1:C:69:TRP:HD1	1.65	0.42
1:E:56:ALA:O	1:E:60:VAL:HG23	2.19	0.42
1:E:144:PRO:HG2	1:E:147:TYR:CB	2.48	0.42
1:E:245:VAL:HG22	1:E:256:ARG:CB	2.49	0.42
1:E:283:SER:OG	1:E:324:GLY:HA3	2.18	0.42
2:I:68:ILE:HD13	2:I:98:PHE:CE1	2.54	0.42
1:C:56:ALA:O	1:C:60:VAL:HG23	2.20	0.42
2:K:38:THR:HG22	2:K:39:ASP:N	2.35	0.42
1:G:173:LEU:HD13	1:G:200:LEU:HD23	2.01	0.42
2:L:77:ASN:HD21	2:L:102:ARG:HE	1.67	0.42
1:A:336:LYS:HG3	1:A:383:GLY:N	2.33	0.42
1:C:80:CYS:HB2	1:C:84:ARG:HG3	2.02	0.42
1:E:173:LEU:HD13	1:E:200:LEU:HD23	2.02	0.42
1:E:180:LYS:HG3	1:E:206:ASP:HB3	2.02	0.42
1:G:97:PRO:C	1:G:99:GLN:H	2.28	0.42
1:A:209:ILE:O	1:A:209:ILE:HG13	2.18	0.42
1:G:180:LYS:HG3	1:G:206:ASP:HB3	2.01	0.42
2:L:68:ILE:HD13	2:L:98:PHE:CE1	2.54	0.42
2:J:68:ILE:HD13	2:J:98:PHE:CE1	2.55	0.42
1:E:340:ASP:O	1:E:344:VAL:HG23	2.20	0.42
1:A:303:TYR:CD1	1:A:304:THR:HG23	2.54	0.42
1:E:79:ALA:C	1:E:80:CYS:SG	3.02	0.42
1:E:285:TRP:CZ3	1:E:291:MET:HG3	2.54	0.42
1:A:153:GLY:C	1:A:324:GLY:HA2	2.45	0.42
1:C:161:GLU:HG3	1:C:292:ILE:HD13	2.02	0.42
2:J:77:ASN:HD21	2:J:102:ARG:HE	1.68	0.42
2:J:104:ALA:O	2:J:106:GLU:N	2.53	0.42
1:E:97:PRO:C	1:E:99:GLN:H	2.28	0.42
1:E:253:MET:HE1	1:E:274:VAL:CG1	2.48	0.42
1:G:56:ALA:O	1:G:60:VAL:HG23	2.20	0.42
1:E:153:GLY:C	1:E:324:GLY:HA2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:TYR:CD1	1:G:267:ILE:HD13	2.55	0.42
1:C:97:PRO:C	1:C:99:GLN:H	2.28	0.41
2:J:38:THR:HG22	2:J:39:ASP:N	2.35	0.41
2:K:104:ALA:O	2:K:106:GLU:N	2.54	0.41
2:L:104:ALA:O	2:L:106:GLU:N	2.53	0.41
1:A:80:CYS:HB2	1:A:84:ARG:HG3	2.03	0.41
2:I:63:GLY:O	2:I:66:MET:HB3	2.21	0.41
2:I:119:ARG:HH21	2:L:44:ARG:HG3	1.85	0.41
1:C:209:ILE:HG13	1:C:209:ILE:O	2.21	0.41
1:C:253:MET:HE1	1:C:274:VAL:CG1	2.50	0.41
1:A:35:LYS:HZ2	1:A:82:MET:HE1	1.81	0.41
1:C:439:ILE:H	1:C:439:ILE:HG13	1.58	0.41
1:G:144:PRO:HG2	1:G:147:TYR:CB	2.50	0.41
1:G:303:TYR:CD1	1:G:304:THR:HG23	2.55	0.41
2:L:108:GLY:O	2:L:128:TYR:HE1	2.03	0.41
2:L:113:ARG:HB3	2:L:121:LEU:HD22	2.01	0.41
1:A:97:PRO:C	1:A:99:GLN:H	2.28	0.41
1:C:154:PRO:HA	1:C:324:GLY:HA2	2.02	0.41
1:C:155:SER:HA	1:C:287:ARG:HD3	2.03	0.41
1:G:253:MET:HE1	1:G:274:VAL:CG1	2.50	0.41
1:A:320:LEU:HD22	1:A:325:VAL:HG21	2.02	0.41
1:A:439:ILE:H	1:A:439:ILE:HG13	1.57	0.41
2:I:102:ARG:O	2:I:103:PRO:C	2.64	0.41
1:C:285:TRP:CZ3	1:C:291:MET:HG3	2.54	0.41
1:C:303:TYR:CD1	1:C:304:THR:HG23	2.55	0.41
1:A:42:LEU:HD13	1:A:139:GLU:HB2	2.02	0.41
1:A:173:LEU:HD13	1:A:200:LEU:HD23	2.03	0.41
1:C:144:PRO:HG2	1:C:147:TYR:CB	2.50	0.41
2:J:102:ARG:O	2:J:103:PRO:C	2.64	0.41
1:A:429:MET:HE1	1:A:446:ILE:HD12	2.03	0.41
1:C:314:ARG:HB3	1:C:347:TYR:CE1	2.56	0.41
1:E:242:TYR:CD1	1:E:267:ILE:HD13	2.56	0.41
2:K:77:ASN:HD21	2:K:102:ARG:HE	1.68	0.41
2:L:33:VAL:HG13	2:L:82:VAL:HG13	2.03	0.41
2:L:38:THR:HG22	2:L:39:ASP:N	2.36	0.41
2:L:102:ARG:O	2:L:103:PRO:C	2.64	0.41
1:A:56:ALA:O	1:A:60:VAL:HG23	2.20	0.41
1:A:154:PRO:HA	1:A:324:GLY:HA2	2.03	0.41
2:L:19:ILE:O	2:L:23:LEU:HG	2.21	0.41
1:A:285:TRP:CZ3	1:A:291:MET:HG3	2.56	0.41
1:A:388:GLN:O	1:A:389:MET:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:82:VAL:CG2	2:J:98:PHE:CE1	3.04	0.41
1:E:39:LEU:HG	1:E:111:PHE:CE1	2.56	0.41
1:G:431:LEU:HD12	2:L:22:GLN:OE1	2.21	0.41
1:A:180:LYS:HG3	1:A:206:ASP:HB3	2.02	0.40
2:I:104:ALA:O	2:I:106:GLU:N	2.54	0.40
1:C:245:VAL:HG13	1:C:245:VAL:O	2.21	0.40
1:E:388:GLN:O	1:E:389:MET:C	2.63	0.40
1:A:254:TYR:OH	1:A:281:SER:HB3	2.20	0.40
1:C:179:PRO:CB	1:C:183:LEU:HD22	2.52	0.40
1:E:80:CYS:HB2	1:E:84:ARG:HG3	2.03	0.40
1:E:209:ILE:O	1:E:209:ILE:HG13	2.21	0.40
2:K:108:GLY:O	2:K:128:TYR:HE1	2.04	0.40
2:K:82:VAL:CG2	2:K:98:PHE:CE1	3.04	0.40
2:K:119:ARG:HD2	2:K:119:ARG:HA	1.85	0.40
1:G:155:SER:HA	1:G:287:ARG:HD3	2.04	0.40
2:L:42:HIS:HB3	2:L:45:ASN:HB2	2.04	0.40
1:A:39:LEU:HG	1:A:111:PHE:CE1	2.56	0.40
1:A:178:LYS:HA	1:A:178:LYS:HD2	1.99	0.40
1:A:274:VAL:HG12	1:A:278:CYS:SG	2.61	0.40
1:A:314:ARG:HB3	1:A:347:TYR:CE1	2.56	0.40
2:I:119:ARG:HA	2:I:119:ARG:HD2	1.82	0.40
2:J:108:GLY:O	2:J:128:TYR:HE1	2.03	0.40
2:K:102:ARG:O	2:K:103:PRO:C	2.64	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	443/485 (91%)	390 (88%)	41 (9%)	12 (3%)	4	10
1	C	443/485 (91%)	389 (88%)	43 (10%)	11 (2%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	443/485 (91%)	390 (88%)	42 (10%)	11 (2%)	4	11
1	G	443/485 (91%)	389 (88%)	44 (10%)	10 (2%)	5	13
2	I	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	2	5
2	J	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	2	5
2	K	127/139 (91%)	104 (82%)	19 (15%)	4 (3%)	3	8
2	L	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	2	5
All	All	2280/2496 (91%)	1974 (87%)	243 (11%)	63 (3%)	4	9

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
2	I	103	PRO
2	I	105	ASP
1	C	207	GLU
2	J	103	PRO
2	J	105	ASP
1	E	207	GLU
2	K	103	PRO
2	K	105	ASP
1	G	207	GLU
2	L	103	PRO
2	L	105	ASP
1	A	81	ASP
1	A	214	PHE
1	A	308	ASN
2	I	56	PHE
1	C	81	ASP
1	C	214	PHE
1	C	308	ASN
2	J	56	PHE
1	E	81	ASP
1	E	214	PHE
1	E	308	ASN
2	K	56	PHE
1	G	81	ASP
1	G	214	PHE
1	G	308	ASN
2	L	56	PHE
1	A	25	MET

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Mol	Chain	Res	Type
1	A	80	CYS
1	A	211	SER
1	C	25	MET
1	C	80	CYS
1	C	211	SER
1	E	25	MET
1	E	80	CYS
1	E	211	SER
1	E	333	ALA
1	G	25	MET
1	G	80	CYS
1	G	211	SER
1	A	333	ALA
1	A	440	LEU
2	I	104	ALA
1	C	333	ALA
1	C	440	LEU
2	J	104	ALA
1	E	440	LEU
2	K	104	ALA
1	G	333	ALA
1	G	440	LEU
2	L	104	ALA
2	I	47	TYR
1	A	66	THR
1	A	371	ALA
1	C	66	THR
2	J	47	TYR
1	E	66	THR
2	L	47	TYR
1	A	334	VAL
1	C	334	VAL
1	E	334	VAL
1	G	334	VAL

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	358/391 (92%)	343 (96%)	15 (4%)	26	55
1	C	358/391 (92%)	343 (96%)	15 (4%)	26	55
1	E	358/391 (92%)	343 (96%)	15 (4%)	26	55
1	G	358/391 (92%)	343 (96%)	15 (4%)	26	55
2	I	115/122 (94%)	106 (92%)	9 (8%)	11	29
2	J	115/122 (94%)	106 (92%)	9 (8%)	11	29
2	K	115/122 (94%)	106 (92%)	9 (8%)	11	29
2	L	115/122 (94%)	106 (92%)	9 (8%)	11	29
All	All	1892/2052 (92%)	1796 (95%)	96 (5%)	21	48

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	39	LEU
1	A	42	LEU
1	A	68	THR
1	A	75	ASP
1	A	80	CYS
1	A	119	LEU
1	A	173	LEU
1	A	183	LEU
1	A	222	LEU
1	A	245	VAL
1	A	271	ASP
1	A	272	LEU
1	A	334	VAL
1	A	377	MET
2	I	10	PHE
2	I	44	ARG
2	I	49	GLU
2	I	59	ARG
2	I	82	VAL
2	I	96	MET
2	I	99	ILE
2	I	103	PRO
2	I	122	ARG
1	C	25	MET
1	C	39	LEU
1	C	42	LEU

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Mol	Chain	Res	Type
1	C	68	THR
1	C	75	ASP
1	C	80	CYS
1	C	119	LEU
1	C	173	LEU
1	C	183	LEU
1	C	222	LEU
1	C	245	VAL
1	C	271	ASP
1	C	272	LEU
1	C	334	VAL
1	C	377	MET
2	J	10	PHE
2	J	44	ARG
2	J	49	GLU
2	J	59	ARG
2	J	82	VAL
2	J	96	MET
2	J	99	ILE
2	J	103	PRO
2	J	122	ARG
1	E	25	MET
1	E	39	LEU
1	E	42	LEU
1	E	68	THR
1	E	75	ASP
1	E	80	CYS
1	E	119	LEU
1	E	173	LEU
1	E	183	LEU
1	E	222	LEU
1	E	245	VAL
1	E	271	ASP
1	E	272	LEU
1	E	334	VAL
1	E	377	MET
2	K	10	PHE
2	K	44	ARG
2	K	49	GLU
2	K	59	ARG
2	K	82	VAL
2	K	96	MET

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Mol	Chain	Res	Type
2	K	99	ILE
2	K	103	PRO
2	K	122	ARG
1	G	25	MET
1	G	39	LEU
1	G	42	LEU
1	G	68	THR
1	G	75	ASP
1	G	80	CYS
1	G	119	LEU
1	G	173	LEU
1	G	183	LEU
1	G	222	LEU
1	G	245	VAL
1	G	271	ASP
1	G	272	LEU
1	G	334	VAL
1	G	377	MET
2	L	10	PHE
2	L	44	ARG
2	L	49	GLU
2	L	59	ARG
2	L	82	VAL
2	L	96	MET
2	L	99	ILE
2	L	103	PRO
2	L	122	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	99	GLN
1	A	208	ASN
1	A	210	ASN
1	A	216	HIS
1	A	229	ASN
1	A	244	ASN
1	A	345	GLN
1	A	385	HIS
1	A	422	ASN
1	A	434	ASN

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Mol	Chain	Res	Type
2	I	18	GLN
2	I	22	GLN
2	I	28	ASN
2	I	45	ASN
2	I	70	ASN
2	I	77	ASN
2	I	78	HIS
2	I	89	HIS
1	C	210	ASN
1	C	216	HIS
1	C	229	ASN
1	C	244	ASN
1	C	345	GLN
1	C	385	HIS
1	C	422	ASN
1	C	434	ASN
2	J	18	GLN
2	J	22	GLN
2	J	28	ASN
2	J	45	ASN
2	J	70	ASN
2	J	77	ASN
2	J	78	HIS
2	J	89	HIS
1	E	96	ASN
1	E	99	GLN
1	E	208	ASN
1	E	210	ASN
1	E	216	HIS
1	E	229	ASN
1	E	244	ASN
1	E	345	GLN
1	E	385	HIS
1	E	422	ASN
1	E	434	ASN
2	K	18	GLN
2	K	22	GLN
2	K	28	ASN
2	K	45	ASN
2	K	70	ASN
2	K	77	ASN
2	K	78	HIS

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Mol	Chain	Res	Type
2	K	89	HIS
1	G	99	GLN
1	G	208	ASN
1	G	210	ASN
1	G	216	HIS
1	G	229	ASN
1	G	244	ASN
1	G	345	GLN
1	G	385	HIS
1	G	422	ASN
1	G	434	ASN
2	L	18	GLN
2	L	22	GLN
2	L	28	ASN
2	L	45	ASN
2	L	70	ASN
2	L	77	ASN
2	L	78	HIS
2	L	89	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
3	PO4	G	507	-	4,4,4	1.82	1 (25%)	6,6,6	1.17	0
3	PO4	C	504	-	4,4,4	1.69	1 (25%)	6,6,6	1.09	0
3	PO4	A	502	-	4,4,4	1.63	1 (25%)	6,6,6	1.11	0
3	PO4	A	501	-	4,4,4	1.77	1 (25%)	6,6,6	1.14	0
3	PO4	E	506	-	4,4,4	1.49	1 (25%)	6,6,6	1.07	0
3	PO4	G	508	-	4,4,4	1.61	1 (25%)	6,6,6	1.18	1 (16%)
3	PO4	C	503	-	4,4,4	1.78	1 (25%)	6,6,6	1.13	0
3	PO4	E	505	-	4,4,4	1.63	1 (25%)	6,6,6	1.16	1 (16%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PO4	P-O3	-3.29	1.45	1.54
3	C	503	PO4	P-O3	-3.28	1.45	1.54
3	G	507	PO4	P-O3	-3.24	1.45	1.54
3	A	502	PO4	P-O3	-3.03	1.45	1.54
3	C	504	PO4	P-O3	-3.03	1.45	1.54
3	E	505	PO4	P-O3	-3.02	1.45	1.54
3	G	508	PO4	P-O3	-2.91	1.46	1.54
3	E	506	PO4	P-O3	-2.70	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	508	PO4	O4-P-O2	2.02	114.20	107.91
3	E	505	PO4	O2-P-O1	-2.01	103.84	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	507	PO4	1	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	445/485 (91%)	0.70	67 (15%) 5 4	2, 29, 99, 100	0
1	C	445/485 (91%)	0.64	55 (12%) 8 7	2, 28, 98, 100	0
1	E	445/485 (91%)	0.82	63 (14%) 6 5	2, 31, 100, 100	0
1	G	445/485 (91%)	0.67	66 (14%) 5 4	2, 26, 98, 100	0
2	I	129/139 (92%)	0.98	22 (17%) 4 3	4, 35, 99, 100	0
2	J	129/139 (92%)	1.15	30 (23%) 2 2	2, 40, 100, 100	0
2	K	129/139 (92%)	1.16	26 (20%) 3 2	3, 41, 98, 100	0
2	L	129/139 (92%)	1.06	26 (20%) 3 2	2, 36, 100, 100	0
All	All	2296/2496 (91%)	0.79	355 (15%) 5 4	2, 31, 100, 100	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	105	ASP	8.6
2	L	98	PHE	7.5
2	L	105	ASP	7.3
1	C	68	THR	7.1
1	G	181	LEU	6.9
1	C	77	LEU	6.9
1	A	68	THR	6.6
1	G	337	LEU	6.0
1	G	77	LEU	6.0
2	K	107	PRO	6.0
1	A	181	LEU	5.9
1	E	181	LEU	5.7
2	J	77	ASN	5.7
2	I	98	PHE	5.7
2	L	107	PRO	5.7
2	I	105	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
2	I	101	ASN	5.4
1	E	339	GLY	5.4
1	E	252	GLU	5.3
1	A	69	TRP	5.3
1	C	337	LEU	5.3
1	G	72	VAL	5.2
1	E	78	THR	5.2
2	K	98	PHE	5.2
1	E	77	LEU	5.1
1	E	72	VAL	5.1
1	E	464	TRP	5.1
1	A	207	GLU	5.0
2	J	105	ASP	4.9
1	E	135	ALA	4.9
1	E	98	GLU	4.9
1	A	339	GLY	4.9
2	L	119	ARG	4.9
1	C	69	TRP	4.8
2	J	108	GLY	4.7
1	G	67	ALA	4.7
1	C	252	GLU	4.7
1	C	66	THR	4.7
1	E	211	SER	4.7
1	E	278	CYS	4.7
1	E	83	TYR	4.7
1	E	71	VAL	4.7
1	G	68	THR	4.6
1	A	74	THR	4.6
1	A	252	GLU	4.5
1	G	22	TYR	4.5
2	I	119	ARG	4.5
1	G	207	GLU	4.5
2	I	107	PRO	4.4
2	L	108	GLY	4.3
1	C	65	SER	4.3
2	K	108	GLY	4.3
1	C	78	THR	4.3
1	G	467	ILE	4.3
1	G	213	PRO	4.3
2	K	38	THR	4.3
1	G	73	TRP	4.3
1	C	467	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
2	J	103	PRO	4.2
1	E	337	LEU	4.2
1	C	338	GLU	4.1
2	J	107	PRO	4.1
2	J	101	ASN	4.1
1	C	466	ASP	4.1
1	G	214	PHE	4.1
2	J	95	VAL	4.1
1	E	66	THR	4.1
1	C	72	VAL	4.1
1	C	79	ALA	4.0
1	G	69	TRP	4.0
1	C	339	GLY	4.0
1	E	28	TRP	4.0
1	E	22	TYR	4.0
1	E	73	TRP	4.0
1	A	210	ASN	4.0
1	E	214	PHE	3.9
1	C	211	SER	3.9
1	C	208	ASN	3.9
1	A	462	ASP	3.9
1	A	464	TRP	3.9
2	J	38	THR	3.8
1	C	181	LEU	3.8
1	E	356	THR	3.8
2	K	90	THR	3.8
1	G	464	TRP	3.8
1	E	65	SER	3.8
1	A	458	ARG	3.8
2	J	129	ALA	3.8
1	G	211	SER	3.7
2	K	91	VAL	3.7
1	E	26	GLY	3.7
1	C	207	GLU	3.7
1	E	207	GLU	3.7
1	A	70	THR	3.6
1	C	180	LYS	3.6
1	A	73	TRP	3.6
1	E	69	TRP	3.6
1	A	77	LEU	3.6
1	A	80	CYS	3.6
1	G	206	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	129	ALA	3.6
1	G	445	GLU	3.5
1	G	372	SER	3.5
2	K	129	ALA	3.5
1	A	76	ARG	3.5
1	E	75	ASP	3.5
1	A	211	SER	3.4
2	K	92	GLU	3.4
2	L	38	THR	3.4
1	A	338	GLU	3.4
1	A	414	GLY	3.4
2	I	43	PRO	3.4
1	E	210	ASN	3.4
1	G	83	TYR	3.4
1	E	68	THR	3.4
1	G	252	GLU	3.4
2	L	103	PRO	3.4
1	E	79	ALA	3.4
2	K	119	ARG	3.4
1	C	210	ASN	3.4
1	C	334	VAL	3.4
1	E	338	GLU	3.3
2	I	103	PRO	3.3
1	A	67	ALA	3.3
1	A	333	ALA	3.3
1	G	131	LYS	3.3
1	G	334	VAL	3.3
1	A	22	TYR	3.3
1	G	339	GLY	3.3
1	G	71	VAL	3.3
1	E	178	LYS	3.2
1	C	83	TYR	3.2
2	J	90	THR	3.2
1	A	214	PHE	3.2
1	G	53	PRO	3.2
1	A	451	ALA	3.2
1	G	210	ASN	3.2
2	J	106	GLU	3.2
1	G	80	CYS	3.2
1	C	464	TRP	3.2
1	G	78	THR	3.2
2	K	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	76	ARG	3.1
1	A	208	ASN	3.1
1	C	98	GLU	3.1
2	L	129	ALA	3.1
1	E	334	VAL	3.1
1	G	458	ARG	3.1
2	I	38	THR	3.1
1	C	439	ILE	3.0
2	J	119	ARG	3.0
1	A	65	SER	3.0
1	G	208	ASN	3.0
2	I	73	ASN	3.0
2	J	73	ASN	3.0
2	K	10	PHE	3.0
1	E	357	GLN	3.0
2	J	44	ARG	3.0
1	E	410	GLY	3.0
1	A	98	GLU	2.9
2	J	21	LYS	2.9
1	C	75	ASP	2.9
1	G	439	ILE	2.9
1	C	381	SER	2.9
1	A	78	THR	2.9
1	A	178	LYS	2.9
2	K	103	PRO	2.9
1	C	31	ASP	2.9
1	C	206	ASP	2.9
2	I	60	ASP	2.9
2	K	95	VAL	2.9
1	C	73	TRP	2.9
1	G	55	GLU	2.8
1	C	76	ARG	2.8
1	A	64	SER	2.8
1	E	70	THR	2.8
1	E	124	ILE	2.8
1	C	178	LYS	2.8
1	G	74	THR	2.8
1	A	31	ASP	2.8
1	E	452	ARG	2.8
1	A	385	HIS	2.8
2	I	91	VAL	2.8
1	A	372	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	413	GLN	2.7
1	C	64	SER	2.7
1	E	208	ASN	2.7
1	A	81	ASP	2.7
1	A	206	ASP	2.7
1	C	287	ARG	2.7
1	E	67	ALA	2.7
2	I	102	ARG	2.7
2	L	7	THR	2.7
2	L	90	THR	2.7
2	I	76	PRO	2.7
1	C	336	LYS	2.7
1	G	307	LYS	2.7
1	E	64	SER	2.7
2	I	92	GLU	2.7
1	G	460	ALA	2.7
2	L	62	ALA	2.7
1	A	467	ILE	2.7
1	C	268	ILE	2.7
2	I	108	GLY	2.7
1	G	98	GLU	2.7
1	A	135	ALA	2.7
1	A	334	VAL	2.7
1	E	467	ILE	2.6
2	L	87	SER	2.6
2	J	7	THR	2.6
2	J	88	THR	2.6
1	A	331	GLY	2.6
1	C	214	PHE	2.6
1	C	274	VAL	2.6
1	G	66	THR	2.6
1	C	22	TYR	2.6
2	L	53	LEU	2.6
1	A	352	ARG	2.6
2	J	92	GLU	2.6
1	A	308	ASN	2.6
2	K	101	ASN	2.6
1	C	74	THR	2.6
2	K	102	ARG	2.6
1	C	465	GLY	2.6
2	L	28	ASN	2.6
2	L	101	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	381	SER	2.5
1	G	178	LYS	2.5
2	J	76	PRO	2.5
1	E	56	ALA	2.5
1	C	82	MET	2.5
1	A	466	ASP	2.5
2	L	60	ASP	2.5
1	A	390	HIS	2.5
1	E	94	PRO	2.5
2	J	98	PHE	2.5
1	E	82	MET	2.5
2	L	1	MET	2.5
2	I	77	ASN	2.5
1	A	75	ASP	2.5
1	E	206	ASP	2.5
1	G	452	ARG	2.5
2	I	70	ASN	2.5
2	I	90	THR	2.5
1	C	278	CYS	2.5
2	J	89	HIS	2.5
2	L	89	HIS	2.5
1	E	336	LYS	2.4
1	G	230	LYS	2.4
1	E	352	ARG	2.4
1	G	26	GLY	2.4
1	C	23	LYS	2.4
2	J	5	GLN	2.4
1	C	374	ARG	2.4
1	A	55	GLU	2.4
1	C	445	GLU	2.4
1	G	49	ASP	2.4
1	A	72	VAL	2.4
1	G	287	ARG	2.4
2	I	59	ARG	2.4
1	A	337	LEU	2.4
1	A	439	ILE	2.4
2	K	70	ASN	2.4
1	A	49	ASP	2.4
1	C	307	LYS	2.4
1	C	213	PRO	2.4
1	A	452	ARG	2.4
1	C	458	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	44	ARG	2.4
2	L	95	VAL	2.4
1	A	100	PHE	2.4
2	K	56	PHE	2.4
1	C	230	LYS	2.3
2	I	21	LYS	2.3
1	G	182	GLY	2.3
1	A	287	ARG	2.3
2	J	102	ARG	2.3
1	G	180	LYS	2.3
1	A	378	PRO	2.3
1	A	26	GLY	2.3
2	J	3	ILE	2.3
1	G	338	GLU	2.3
1	E	372	SER	2.3
1	G	413	GLN	2.3
1	E	33	VAL	2.3
1	G	60	VAL	2.3
2	J	56	PHE	2.3
1	A	415	ILE	2.3
2	I	89	HIS	2.3
1	G	70	THR	2.3
1	G	336	LYS	2.3
1	A	130	PHE	2.3
1	A	278	CYS	2.2
1	A	66	THR	2.2
2	L	88	THR	2.2
2	K	73	ASN	2.2
2	L	102	ARG	2.2
1	E	60	VAL	2.2
1	G	87	ALA	2.2
2	L	46	THR	2.2
1	A	95	ASN	2.2
2	L	76	PRO	2.2
1	E	48	GLN	2.2
2	J	57	ASP	2.2
1	A	230	LYS	2.2
2	K	100	VAL	2.2
1	C	67	ALA	2.2
1	E	340	ASP	2.2
2	J	91	VAL	2.2
1	A	268	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	135	ALA	2.2
1	A	442	GLU	2.2
2	K	17	GLU	2.2
2	K	46	THR	2.2
1	E	126	ASN	2.2
1	A	131	LYS	2.2
2	L	127	SER	2.2
1	C	304	THR	2.1
1	E	76	ARG	2.1
1	G	352	ARG	2.1
1	G	278	CYS	2.1
2	K	76	PRO	2.1
1	G	86	LYS	2.1
1	G	441	ASN	2.1
1	G	82	MET	2.1
1	G	183	LEU	2.1
2	L	58	LEU	2.1
1	E	133	ILE	2.1
1	E	411	HIS	2.1
1	G	127	VAL	2.1
1	E	306	GLN	2.1
1	E	440	LEU	2.1
2	J	78	HIS	2.1
2	K	89	HIS	2.1
1	G	85	ALA	2.1
1	G	84	ARG	2.1
1	A	395	LEU	2.1
1	E	198	GLY	2.1
1	E	439	ILE	2.1
1	G	75	ASP	2.1
1	E	445	GLU	2.1
2	K	59	ARG	2.1
1	A	28	TRP	2.1
2	K	20	THR	2.1
1	E	25	MET	2.1
1	C	198	GLY	2.1
1	A	52	ASP	2.0
1	G	36	ASP	2.0
2	J	59	ARG	2.0
1	G	117	ALA	2.0
1	A	134	LYS	2.0
1	C	409	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	268	ILE	2.0
1	G	273	ILE	2.0
2	J	6	GLY	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(Å ²)	Q<0.9
3	PO4	G	508	5/5	0.77	0.22	18,23,40,42	0
3	PO4	E	506	5/5	0.81	0.24	18,23,40,42	0
3	PO4	C	504	5/5	0.84	0.20	18,23,40,42	0
3	PO4	C	503	5/5	0.90	0.20	18,23,40,42	0
3	PO4	A	502	5/5	0.90	0.17	18,23,40,42	0
3	PO4	E	505	5/5	0.93	0.21	18,23,40,42	0
3	PO4	G	507	5/5	0.94	0.15	18,23,40,42	0
3	PO4	A	501	5/5	0.94	0.18	18,23,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.