



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:41 PM GMT

PDB ID : 1BXN
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

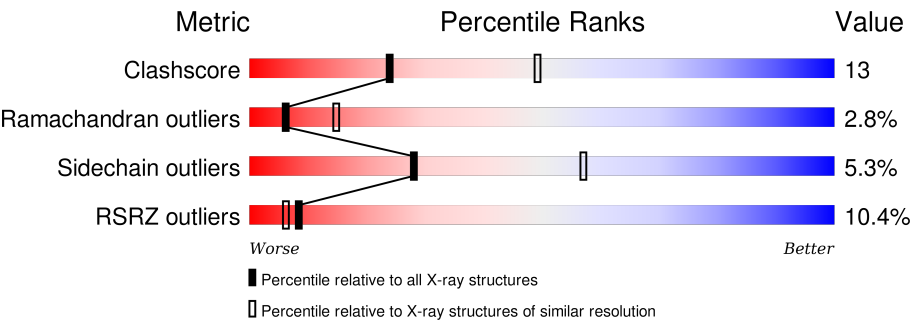
1 Overall quality at a glance i

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>8%</div><div>65%24%8%</div></div>
1	C	485	<div><div>9%</div><div>65%24%8%</div></div>
1	E	485	<div><div>11%</div><div>65%24%8%</div></div>
1	G	485	<div><div>8%</div><div>66%23%8%</div></div>
2	I	139	<div><div>12%</div><div>55%33%5%7%</div></div>
2	J	139	<div><div>12%</div><div>53%35%5%7%</div></div>
2	K	139	<div><div>11%</div><div>53%35%7%</div></div>

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Mol	Chain	Length	Quality of chain
2	L	139	 A horizontal bar chart showing the quality of chain L. The bar is divided into five segments: red (12%), green (50%), yellow (37%), orange (5%), and grey (7%). The segments are labeled with their respective percentages: 12%, 50%, 37%, 5%, and 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 (three-letter code: PO4) (formula: O₄P).

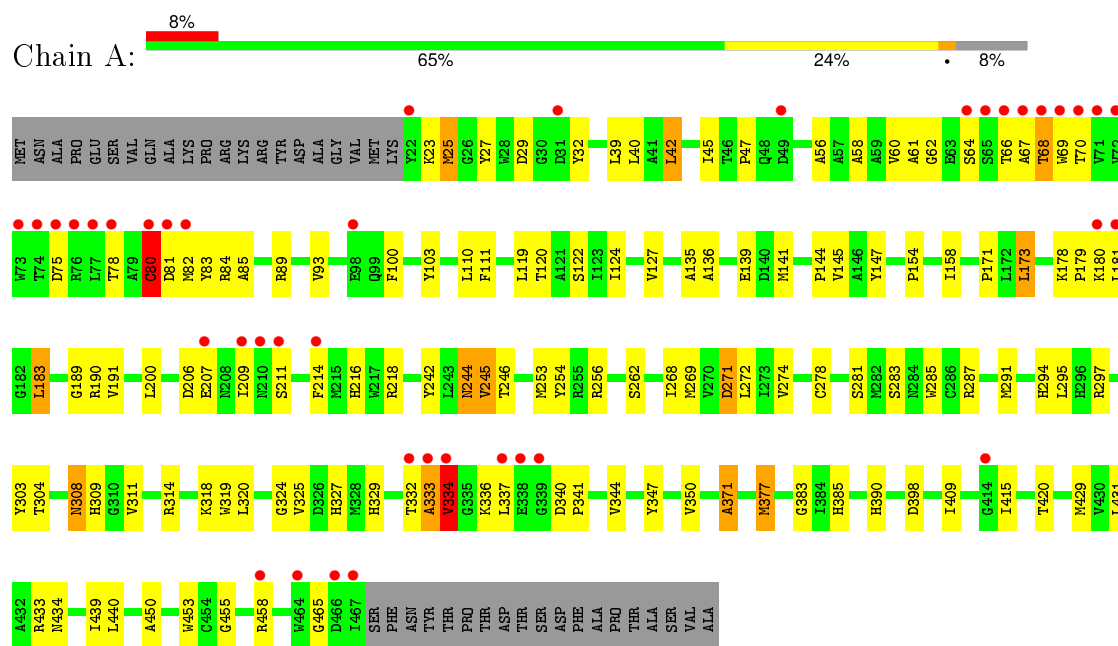


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

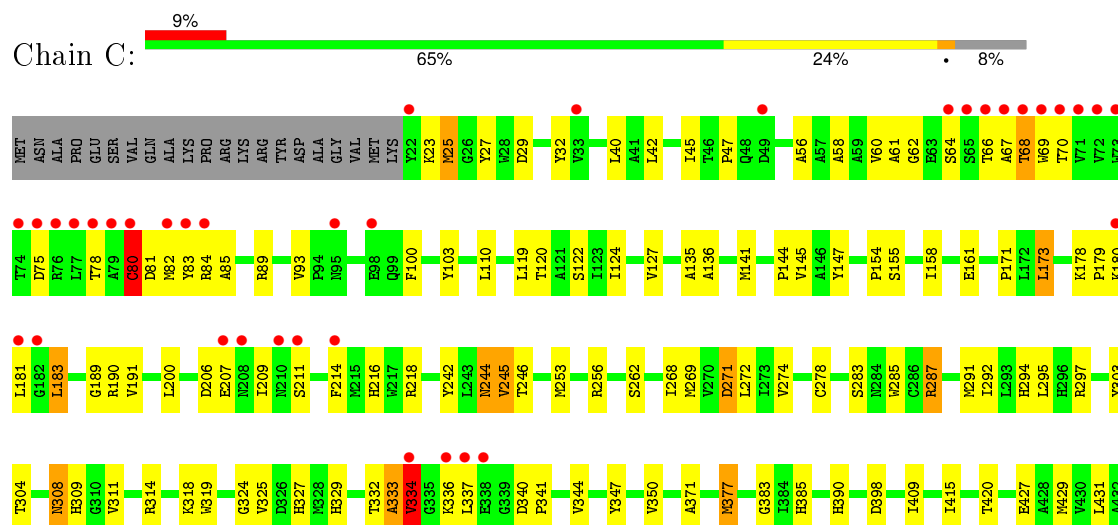
3 Residue-property plots [i](#)

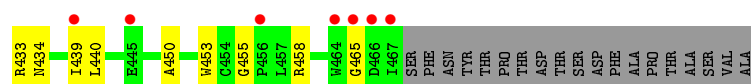
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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)

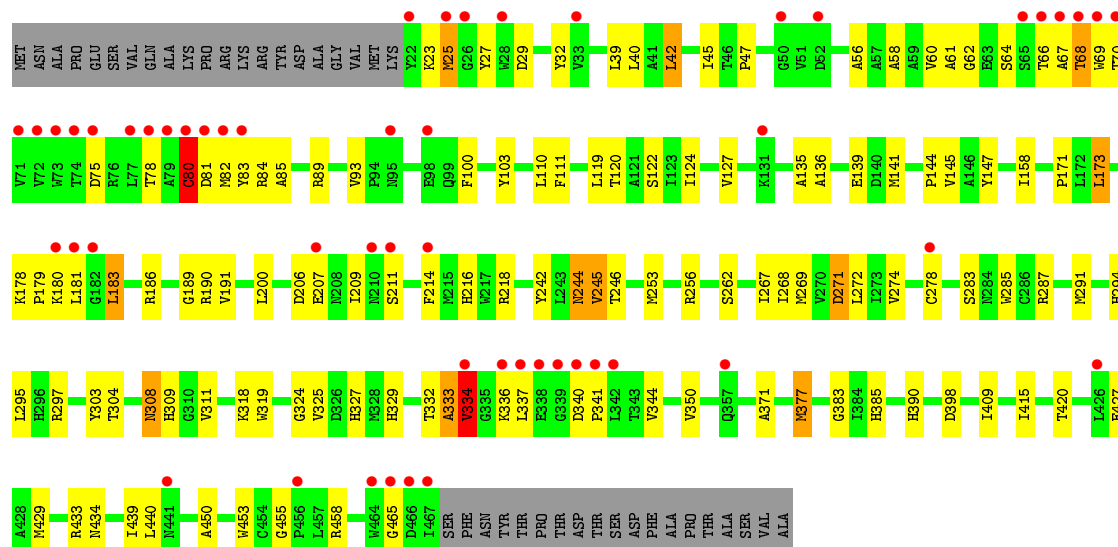


• Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)

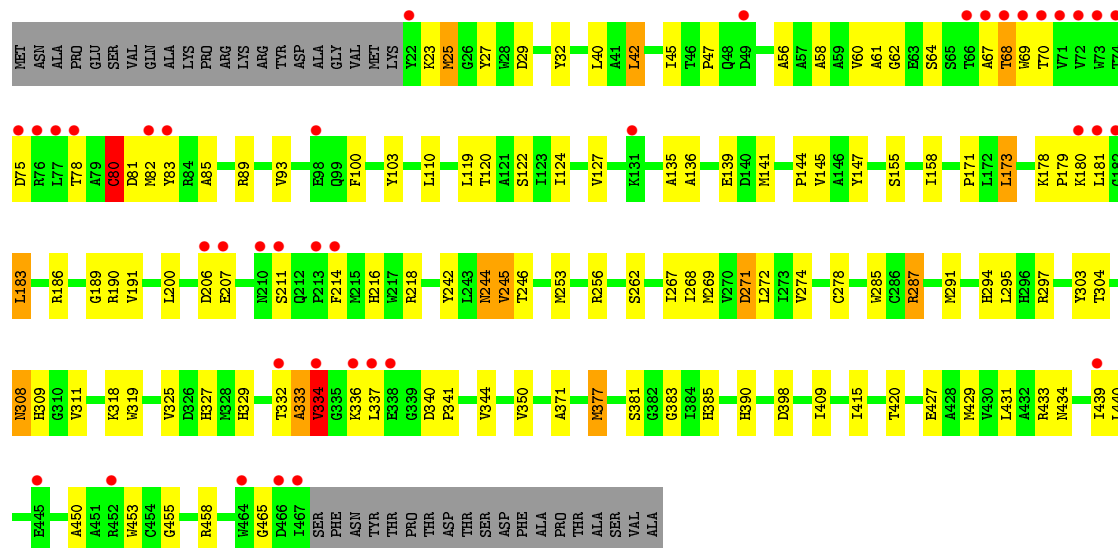




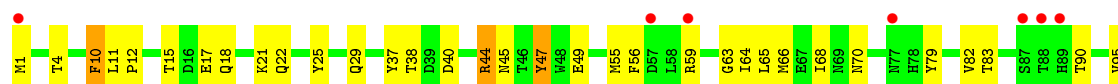
• Molecule 1: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN)



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

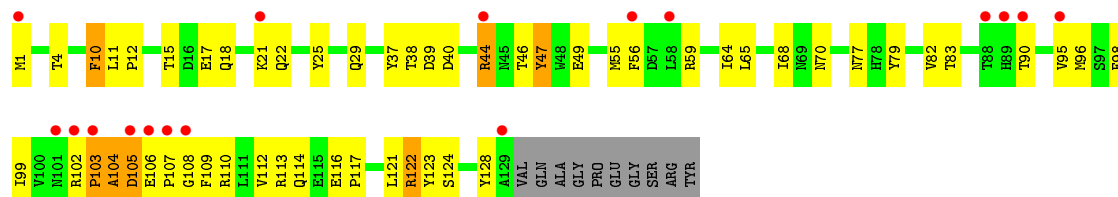


• Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)

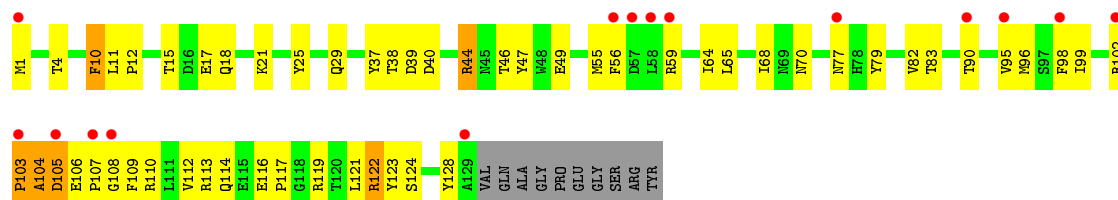




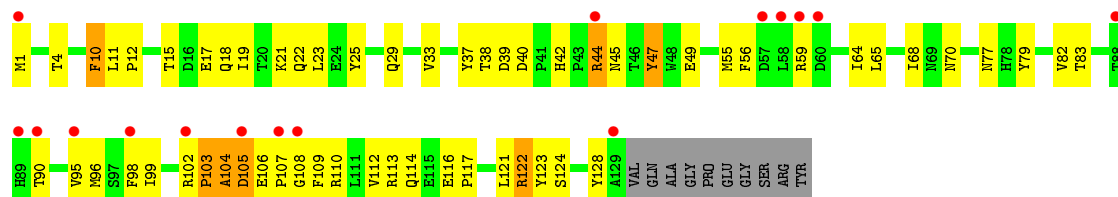
● Molecule 2: PROTEIN (RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN)



● 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	112.00 Å 112.00 Å 402.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 24.60 – 2.65	Depositor EDS
% Data completeness (in resolution range)	90.0 (15.00-2.70) 86.9 (24.60-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.64 Å)	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.	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65682 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/3552	0.57	0/4816
1	C	0.33	0/3552	0.57	0/4816
1	E	0.33	0/3552	0.57	0/4816
1	G	0.34	0/3552	0.57	0/4816
2	I	0.37	0/1084	0.61	0/1474
2	J	0.36	0/1084	0.61	0/1474
2	K	0.36	0/1084	0.61	0/1474
2	L	0.36	0/1084	0.61	0/1474
All	All	0.34	0/18544	0.58	0/25160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	89	0
1	C	3470	0	3402	88	0
1	E	3470	0	3402	86	0
1	G	3470	0	3402	84	0
2	I	1056	0	1007	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1056	0	1007	39	0
2	K	1056	0	1007	39	0
2	L	1056	0	1007	42	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	467	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 13.

All (467) 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: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
2:K:104:ALA:O	2:K:107:PRO:HD3	1.89	0.73
1:C:245:VAL:HG21	1:C:268:ILE:HD11	1.71	0.73
1:G:420:THR:HG23	2:L:10:PHE:HE2	1.54	0.72
1:G:245:VAL:HG21	1:G:268:ILE:HD11	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:112:VAL:HB	2:L:124:SER:HB2	1.72	0.70
2:K:25:TYR:O	2:K:29:GLN:HG2	1.91	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
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
1:A:297:ARG:HG2	1:A:329:HIS:HB2	1.74	0.69
2:I:25:TYR:O	2:I:29:GLN:HG2	1.93	0.69
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:334:VAL:HB	1:C:341:PRO:HG3	1.82	0.62
1:G:242:TYR:HB3	1:G:269:MET:HB2	1.82	0.61
1:G:274:VAL:HG12	1:G:278:CYS:CB	2.30	0.61
1:E:180:LYS:HG2	1:E:181:LEU:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:274:VAL:HG12	1:A:278:CYS:CB	2.30	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
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
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:E:61:ALA:HB1	1:E:85:ALA:O	2.03	0.59
2:J:44:ARG:HA	2:J:44:ARG:HH11	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:333:ALA:HB2	1:C:344:VAL:HG11	1.86	0.58
1:C:61:ALA:HB1	1:C:85:ALA:O	2.04	0.58
2:K:44:ARG:HH11	2:K:44:ARG:HA	1.66	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
2:J:90:THR:HB	1:E:183:LEU:HA	1.87	0.57
1:A:333:ALA:HB2	1:A:344:VAL:HG11	1.87	0.57
1:A:189:GLY:HA3	2:L:47:TYR:OH	2.05	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:433:ARG:NH2	1:A:434:ASN:HD21	2.02	0.57
1:A:68:THR:HG23	1:A:70:THR:O	2.05	0.57
1:C:68:THR:HG23	1:C:70:THR:O	2.05	0.57
1:E:245:VAL:HG22	1:E:256:ARG:HB2	1.87	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
2:I:44:ARG:HA	2:I:44:ARG:HH11	1.68	0.57
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: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: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:145:VAL:HG13	1:E:371:ALA:HB2	1.86	0.56
1:E:136:ALA:O	1:E:309:HIS:HA	2.05	0.56
1:G:433:ARG:HG3	1:G:439:ILE:HD11	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: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:E:433:ARG:NH2	1:E:434:ASN:HD21	2.02	0.56
1:E:420:THR:HG23	2:K:10:PHE:CE2	2.36	0.56
1:A:23:LYS:HA	1:A:58:ALA:HB1	1.86	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:G:433:ARG:NH2	1:G:434:ASN:HD21	2.02	0.55
1:A:337:LEU:HD22	1:A:337:LEU:H	1.71	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
1:G:333:ALA:HB2	1:G:344:VAL:HG11	1.88	0.55
2:J:82:VAL:HG23	2:J:98:PHE:CE1	2.42	0.55
1:C:93:VAL:HG23	1:C:100:PHE:HA	1.88	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:A:216:HIS:HD2	1:A:218:ARG:HB2	1.72	0.55
1:C:245:VAL:HG22	1:C:256:ARG:HB2	1.87	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:A:93:VAL:HG23	1:A:100:PHE:HA	1.88	0.55
1:C:23:LYS:HA	1:C:58:ALA:HB1	1.87	0.55
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
2:J:82:VAL:HG23	2:J:98:PHE:HE1	1.71	0.54
1:A:136:ALA:O	1:A:309:HIS:HA	2.07	0.54
1:G:216:HIS:HD2	1:G:218:ARG:HB2	1.72	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:C:179:PRO:HG2	1:C:191:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:HIS:HD2	1:E:218:ARG:HB2	1.72	0.54
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
1:C:337:LEU:HD22	1:C:337:LEU:H	1.73	0.53
2:K:82:VAL:HG23	2:K:98:PHE:CE1	2.43	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:H	1:E:337:LEU:HD22	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
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
2:K:1:MET:SD	2:K:107:PRO:HD2	2.48	0.53
1:C:274:VAL:HG12	1:C:278:CYS:HB2	1.89	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:E:333:ALA:HB2	1:E:344:VAL:HG11	1.90	0.52
1:C:216:HIS:HD2	1:C:218:ARG:HB2	1.74	0.52
2:I:1:MET:SD	2:I:107:PRO:HD2	2.49	0.52
2:L:82:VAL:HG23	2:L:98:PHE:CE1	2.43	0.52
2:J:114:GLN:HB3	2:J:122:ARG:HB3	1.92	0.52
2:I:114:GLN:HB3	2:I:122:ARG:HB3	1.92	0.52
1:A:318:LYS:HG2	1:A:350:VAL:HG13	1.92	0.52
1:G:179:PRO:HG2	1:G:191:VAL:HG21	1.91	0.52
1:C:83:TYR:HA	1:C:110:LEU:HD21	1.92	0.52
1:G:381:SER:HB3	3:G:507:PO4:O3	2.10	0.52
2:K:104:ALA:HB1	2:K:107:PRO:HG3	1.92	0.52
1:C:294:HIS:HA	1:C:327:HIS:HB2	1.92	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
2:J:1:MET:SD	2:J:107:PRO:HD2	2.50	0.51
1:A:294:HIS:HA	1:A:327:HIS:HB2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:64:SER:HB2	1:G:122:SER:O	2.11	0.51
2:L:104:ALA:HB1	2:L:107:PRO:HG3	1.92	0.51
2:J:47:TYR:OH	1:E:189:GLY:HA3	2.10	0.51
2:K:17:GLU:O	2:K:21:LYS:HG3	2.11	0.50
1:E:295:LEU:HB2	1:E:325:VAL:CG1	2.41	0.50
1:C:295:LEU:HB2	1:C:325:VAL:CG1	2.42	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: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
2:L:1:MET:SD	2:L:107:PRO:HD2	2.51	0.50
1:E:64:SER:HB2	1:E:122:SER:O	2.11	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:G:333:ALA:O	1:G:334:VAL:HG12	2.13	0.49
1:C:318:LYS:HG2	1:C:350:VAL:HG13	1.93	0.49
2:L:4:THR:O	2:L:4:THR:HG22	2.13	0.49
1:G:178:LYS:HB3	1:G:409:ILE:HG21	1.94	0.49
2:K:4:THR:HG22	2:K:4:THR:O	2.12	0.49
2:L:17:GLU:O	2:L:21:LYS:HG3	2.13	0.49
1:G:271:ASP:O	1:G:274:VAL:HG23	2.13	0.49
1:A:333:ALA:O	1:A:334:VAL:HG12	2.13	0.49
1:G:295:LEU:HB2	1:G:325:VAL:CG1	2.43	0.49
1:G:27:TYR:CZ	1:G:67:ALA:HB2	2.48	0.48
1:A:29:ASP:HB3	1:A:32:TYR:HB2	1.95	0.48
1:A:429:MET:HE2	1:A:439:ILE:HG23	1.94	0.48
2:K:116:GLU:HB3	2:K:117:PRO:HD2	1.94	0.48
1:A:178:LYS:HB3	1:A:409:ILE:HG21	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:J:112:VAL:O	2:J:123:TYR:HA	2.12	0.48
1:G:89:ARG:HB2	1:G:103:TYR:HB2	1.96	0.48
2:I:4:THR:O	2:I:4:THR:HG22	2.14	0.48
1:G:120:THR:HG22	1:G:319:TRP:CH2	2.48	0.48
1:C:89:ARG:HB2	1:C:103:TYR:HB2	1.96	0.48
1:G:40:LEU:O	1:G:141:MET:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:MET:CE	1:C:439:ILE:HG23	2.44	0.48
1:A:271:ASP:O	1:A:274:VAL:HG23	2.13	0.48
1:A:64:SER:HB2	1:A:122:SER:O	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:E:333:ALA:O	1:E:334:VAL:HG12	2.13	0.48
1:C:64:SER:HB2	1:C:122:SER:O	2.13	0.48
1:C:27:TYR:CZ	1:C:67:ALA:HB2	2.49	0.48
1:E:295:LEU:HB2	1:E:325:VAL:HG11	1.96	0.48
2:I:117:PRO:HB3	1:G:262:SER:HA	1.95	0.48
1:C:178:LYS:HB3	1:C:409:ILE:HG21	1.96	0.48
1:C:245:VAL:HG13	1:C:253:MET:HG3	1.96	0.47
1:E:83:TYR:HA	1:E:110:LEU:HD21	1.95	0.47
2:I:17:GLU:O	2:I:21:LYS:HG3	2.14	0.47
2:J:17:GLU:O	2:J:21:LYS:HG3	2.14	0.47
1:A:83:TYR:HA	1:A:110:LEU:HD21	1.95	0.47
2:J:4:THR:HG22	2:J:4:THR:O	2.14	0.47
1:G:244:ASN:ND2	1:G:246:THR:H	2.12	0.47
1:C:144:PRO:HG2	1:C:147:TYR:HB2	1.97	0.47
1:A:124:ILE:O	1:A:127:VAL:HG22	2.14	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
2:L:112:VAL:O	2:L:123:TYR:HA	2.14	0.47
1:C:124:ILE:O	1:C:127:VAL:HG22	2.14	0.47
1:E:27:TYR:CZ	1:E:67:ALA:HB2	2.50	0.47
1:A:27:TYR:CZ	1:A:67:ALA:HB2	2.49	0.47
1:C:29:ASP:HB3	1:C:32:TYR:HB2	1.97	0.47
1:A:89:ARG:HB2	1:A:103:TYR:HB2	1.96	0.47
1:E:433:ARG:HG3	1:E:439:ILE:CD1	2.45	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: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:333:ALA:O	1:C:334:VAL:HG12	2.14	0.47
1:G:120:THR:HG22	1:G:319:TRP:CZ3	2.50	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
2:J:46:THR:HG21	1:E:186:ARG:HG3	1.96	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:C:244:ASN:ND2	1:C:246:THR:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:THR:HG22	1:E:319:TRP:CH2	2.50	0.46
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:A:120:THR:HG22	1:A:319:TRP:CH2	2.51	0.46
1:E:271:ASP:O	1:E:274:VAL:HG23	2.15	0.46
1:C:450:ALA:HA	1:C:453:TRP:NE1	2.31	0.46
1:C:390:HIS:CD2	1:C:390:HIS:H	2.34	0.46
1:E:429:MET:CE	1:E:439:ILE:HG23	2.46	0.46
1:E:120:THR:HG22	1:E:319:TRP:CZ3	2.50	0.46
1:A:431:LEU:HD12	2:I:22:GLN:OE1	2.15	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:E:415:ILE:H	1:E:415:ILE:HD12	1.81	0.46
1:A:80:CYS:O	1:A:82:MET:N	2.49	0.46
1:A:433:ARG:HG3	1:A:439:ILE:CD1	2.46	0.46
1:A:245:VAL:HG13	1:A:253:MET:HG3	1.97	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
2:K:112:VAL:O	2:K:123:TYR:HA	2.16	0.46
1:A:262:SER:HA	2:J:117:PRO:HB3	1.98	0.46
1:G:450:ALA:HA	1:G:453:TRP:NE1	2.31	0.46
1:E:29:ASP:HB3	1:E:32:TYR:HB2	1.97	0.46
1:G:429:MET:CE	1:G:439:ILE:HG23	2.46	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
2:K:65:LEU:HA	2:K:68:ILE:HD12	1.99	0.45
1:A:244:ASN:ND2	1:A:246:THR:H	2.15	0.45
1:A:171:PRO:HA	1:A:398:ASP:O	2.15	0.45
1:G:285:TRP:CZ3	1:G:291:MET:HG3	2.51	0.45
1:G:69:TRP:H	1:G:69:TRP:HD1	1.64	0.45
1:G:42:LEU:HD13	1:G:139:GLU:HB2	1.98	0.45
1:E:450:ALA:HA	1:E:453:TRP:NE1	2.31	0.45
1:E:429:MET:HE2	1:E:439:ILE:HG23	1.98	0.45
2:K:46:THR:HG21	1:G:186:ARG:HG3	1.97	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
1:G:171:PRO:HA	1:G:398:ASP:O	2.16	0.45
1:A:450:ALA:HA	1:A:453:TRP:NE1	2.31	0.45
1:A:390:HIS:H	1:A:390:HIS:CD2	2.35	0.45
1:E:455:GLY:O	1:E:458:ARG:HB3	2.16	0.45
1:C:429:MET:HE2	1:C:439:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:HG22	1:C:319:TRP:CZ3	2.51	0.45
1:E:135:ALA:HB1	1:E:308:ASN:O	2.17	0.45
2:I:109:PHE:HD1	2:I:109:PHE:H	1.64	0.45
1:E:69:TRP:H	1:E:69:TRP:HD1	1.65	0.45
2:L:65:LEU:HA	2:L:68:ILE:HD12	1.97	0.45
1:C:40:LEU:O	1:C:141:MET:HA	2.16	0.45
1:A:415:ILE:H	1:A:415:ILE:HD12	1.81	0.45
1:A:40:LEU:O	1:A:141:MET:HA	2.16	0.45
1:C:80:CYS:O	1:C:82:MET:N	2.50	0.45
1:E:390:HIS:H	1:E:390:HIS:CD2	2.35	0.45
1:G:144:PRO:HG2	1:G:147:TYR:HB2	1.98	0.45
1:C:45:ILE:HG22	1:C:47:PRO:HD3	1.98	0.45
1:G:429:MET:HE2	1:G:439:ILE:HG23	1.98	0.44
1:A:429:MET:CE	1:A:439:ILE:HG23	2.46	0.44
1:E:385:HIS:HE1	1:E:465:GLY:O	2.00	0.44
1:C:455:GLY:O	1:C:458:ARG:HB3	2.17	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
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
2:J:109:PHE:H	2:J:109:PHE:HD1	1.66	0.44
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:G:245:VAL:HG13	1:G:253:MET:HG3	1.99	0.44
1:E:336:LYS:HG3	1:E:383:GLY:N	2.33	0.44
2:J:37:TYR:HA	2:J:79:TYR:O	2.18	0.44
1:C:173:LEU:HD13	1:C:200:LEU:HD23	1.99	0.44
1:G:80:CYS:O	1:G:82:MET:N	2.51	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: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:431:LEU:HD12	2:J:22:GLN:OE1	2.18	0.44
1:C:427:GLU:HG3	2:J:10:PHE:HB2	2.00	0.44
2:J:104:ALA:O	2:J:105:ASP:C	2.55	0.44
2:J:65:LEU:HA	2:J:68:ILE:HD12	1.98	0.44
1:G:427:GLU:HG3	2:L:10:PHE:HB2	2.00	0.44
1:C:340:ASP:O	1:C:344:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:GLY:O	1:G:458:ARG:HB3	2.17	0.44
1:E:439:ILE:HG13	1:E:439:ILE:H	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:G:336:LYS:HG3	1:G:383:GLY:N	2.33	0.43
1:A:385:HIS:HE1	1:A:465:GLY:O	2.00	0.43
1:A:283:SER:OG	1:A:324:GLY:HA3	2.18	0.43
1:G:433:ARG:HG3	1:G:439:ILE:CD1	2.47	0.43
2:K:104:ALA:O	2:K:105:ASP:C	2.56	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:C:336:LYS:HG3	1:C:383:GLY:N	2.33	0.43
1:C:283:SER:OG	1:C:324:GLY:HA3	2.18	0.43
1:C:135:ALA:HB1	1:C:308:ASN:O	2.19	0.43
2:I:37:TYR:HA	2:I:79:TYR:O	2.18	0.43
1:G:415:ILE:HD12	1:G:415:ILE:H	1.84	0.43
2:K:109:PHE:H	2:K:109:PHE:HD1	1.64	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
2:L:37:TYR:HA	2:L:79:TYR:O	2.18	0.43
1:A:69:TRP:HD1	1:A:69:TRP:H	1.66	0.43
1:G:295:LEU:CB	1:G:325:VAL:HG11	2.49	0.43
2:I:113:ARG:HH22	2:L:45:ASN:ND2	2.17	0.43
2:K:113:ARG:HB3	2:K:121:LEU:HD22	2.01	0.43
1:A:135:ALA:HB1	1:A:308:ASN:O	2.19	0.43
2:K:90:THR:HG21	1:G:183:LEU:HG	2.01	0.43
2:K:68:ILE:HD13	2:K:98:PHE:CE1	2.53	0.43
1:A:144:PRO:HG2	1:A:147:TYR:CB	2.49	0.43
2:L:104:ALA:O	2:L:105:ASP:C	2.56	0.42
1:E:245:VAL:HG22	1:E:256:ARG:CB	2.49	0.42
2:I:104:ALA:O	2:I:105:ASP:C	2.56	0.42
1:E:144:PRO:HG2	1:E:147:TYR:CB	2.48	0.42
1:E:56:ALA:O	1:E:60:VAL:HG23	2.19	0.42
1:E:283:SER:OG	1:E:324:GLY:HA3	2.18	0.42
1:C:69:TRP:H	1:C:69:TRP:HD1	1.65	0.42
2:I:68:ILE:HD13	2:I:98:PHE:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ALA:O	1:C:60:VAL:HG23	2.20	0.42
1:A:336:LYS:HG3	1:A:383:GLY:N	2.33	0.42
1:E:180:LYS:HG3	1:E:206:ASP:HB3	2.02	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: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
1:A:209:ILE:HG13	1:A:209:ILE:O	2.18	0.42
1:E:340:ASP:O	1:E:344:VAL:HG23	2.20	0.42
2:J:68:ILE:HD13	2:J:98:PHE:CE1	2.55	0.42
1:A:303:TYR:CD1	1:A:304:THR:HG23	2.54	0.42
1:E:285:TRP:CZ3	1:E:291:MET:HG3	2.54	0.42
2:J:104:ALA:O	2:J:106:GLU:N	2.53	0.42
2:J:77:ASN:HD21	2:J:102:ARG:HE	1.68	0.42
1:C:161:GLU:HG3	1:C:292:ILE:HD13	2.02	0.42
1:G:56:ALA:O	1:G:60:VAL:HG23	2.20	0.42
1:G:242:TYR:CD1	1:G:267:ILE:HD13	2.55	0.42
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
2:I:119:ARG:HH21	2:L:44:ARG:HG3	1.85	0.41
1:A:80:CYS:HB2	1:A:84:ARG:HG3	2.03	0.41
1:C:209:ILE:O	1:C:209:ILE:HG13	2.21	0.41
2:I:63:GLY:O	2:I:66:MET:HB3	2.21	0.41
1:E:78:THR:C	1:E:80:CYS:H	2.24	0.41
1:C:439:ILE:HG13	1:C:439:ILE:H	1.58	0.41
1:G:303:TYR:CD1	1:G:304:THR:HG23	2.55	0.41
1:C:78:THR:C	1:C:80:CYS:H	2.24	0.41
1:G:144:PRO:HG2	1:G:147:TYR:CB	2.50	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: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:A:439:ILE:H	1:A:439:ILE:HG13	1.57	0.41
1:C:303:TYR:CD1	1:C:304:THR:HG23	2.55	0.41
1:A:320:LEU:HD22	1:A:325:VAL:HG21	2.02	0.41
1:C:285:TRP:CZ3	1:C:291:MET:HG3	2.54	0.41
1:C:144:PRO:HG2	1:C:147:TYR:CB	2.50	0.41
1:A:173:LEU:HD13	1:A:200:LEU:HD23	2.03	0.41
1:A:42:LEU:HD13	1:A:139:GLU:HB2	2.02	0.41
2:L:38:THR:HG22	2:L:39:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:TYR:CD1	1:E:267:ILE:HD13	2.56	0.41
2:L:33:VAL:HG13	2:L:82:VAL:HG13	2.03	0.41
1:C:314:ARG:HB3	1:C:347:TYR:CE1	2.56	0.41
2:K:77:ASN:HD21	2:K:102:ARG:HE	1.68	0.41
1:A:78:THR:C	1:A:80:CYS:H	2.24	0.41
1:G:78:THR:C	1:G:80:CYS:H	2.24	0.41
1:A:154:PRO:HA	1:A:324:GLY:HA2	2.03	0.41
1:A:56:ALA:O	1:A:60:VAL:HG23	2.20	0.41
2:L:19:ILE:O	2:L:23:LEU:HG	2.21	0.41
2:J:82:VAL:CG2	2:J:98:PHE:CE1	3.04	0.41
1:A:285:TRP:CZ3	1:A:291:MET:HG3	2.56	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
2:I:104:ALA:O	2:I:106:GLU:N	2.54	0.40
1:A:180:LYS:HG3	1:A:206:ASP:HB3	2.02	0.40
1:C:245:VAL:O	1:C:245:VAL:HG13	2.21	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:A:254:TYR:OH	1:A:281:SER:HB3	2.20	0.40
2:K:108:GLY:O	2:K:128:TYR:HE1	2.04	0.40
1:E:209:ILE:HG13	1:E:209:ILE:O	2.21	0.40
2:K:82:VAL:CG2	2:K:98:PHE:CE1	3.04	0.40
2:L:42:HIS:HB3	2:L:45:ASN:HB2	2.04	0.40
1:G:155:SER:HA	1:G:287:ARG:HD3	2.04	0.40
2:K:119:ARG:HA	2:K:119:ARG:HD2	1.85	0.40
1:A:274:VAL:HG12	1:A:278:CYS:SG	2.61	0.40
2:I:119:ARG:HD2	2:I:119:ARG:HA	1.82	0.40
1:A:178:LYS:HA	1:A:178:LYS:HD2	1.99	0.40
1:A:314:ARG:HB3	1:A:347:TYR:CE1	2.56	0.40
2:J:108:GLY:O	2:J:128:TYR:HE1	2.03	0.40
1:A:39:LEU:HG	1:A:111:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	6	16
1	C	443/485 (91%)	389 (88%)	43 (10%)	11 (2%)	7	18
1	E	443/485 (91%)	390 (88%)	42 (10%)	11 (2%)	7	18
1	G	443/485 (91%)	389 (88%)	44 (10%)	10 (2%)	8	20
2	I	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	4	8
2	J	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	4	8
2	K	127/139 (91%)	104 (82%)	19 (15%)	4 (3%)	5	12
2	L	127/139 (91%)	104 (82%)	18 (14%)	5 (4%)	4	8
All	All	2280/2496 (91%)	1974 (87%)	243 (11%)	63 (3%)	6	15

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

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Mol	Chain	Res	Type
1	G	81	ASP
1	G	214	PHE
1	G	308	ASN
2	L	56	PHE
1	A	25	MET
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%)	36	68
1	C	358/391 (92%)	343 (96%)	15 (4%)	36	68
1	E	358/391 (92%)	343 (96%)	15 (4%)	36	68
1	G	358/391 (92%)	343 (96%)	15 (4%)	36	68
2	I	115/122 (94%)	105 (91%)	10 (9%)	13	29
2	J	115/122 (94%)	105 (91%)	10 (9%)	13	29
2	K	115/122 (94%)	105 (91%)	10 (9%)	13	29
2	L	115/122 (94%)	105 (91%)	10 (9%)	13	29
All	All	1892/2052 (92%)	1792 (95%)	100 (5%)	28	57

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
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	244	ASN
1	A	245	VAL
1	A	271	ASP
1	A	272	LEU
1	A	287	ARG
1	A	334	VAL
1	A	377	MET
2	I	10	PHE
2	I	44	ARG
2	I	49	GLU
2	I	59	ARG

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Mol	Chain	Res	Type
2	I	70	ASN
2	I	96	MET
2	I	99	ILE
2	I	103	PRO
2	I	110	ARG
2	I	122	ARG
1	C	25	MET
1	C	42	LEU
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	244	ASN
1	C	245	VAL
1	C	271	ASP
1	C	272	LEU
1	C	287	ARG
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	70	ASN
2	J	96	MET
2	J	99	ILE
2	J	103	PRO
2	J	110	ARG
2	J	122	ARG
1	E	25	MET
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	244	ASN
1	E	245	VAL
1	E	271	ASP

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Mol	Chain	Res	Type
1	E	272	LEU
1	E	287	ARG
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	70	ASN
2	K	96	MET
2	K	99	ILE
2	K	103	PRO
2	K	110	ARG
2	K	122	ARG
1	G	25	MET
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	244	ASN
1	G	245	VAL
1	G	271	ASP
1	G	272	LEU
1	G	287	ARG
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	70	ASN
2	L	96	MET
2	L	99	ILE
2	L	103	PRO
2	L	110	ARG
2	L	122	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	216	HIS
1	A	244	ASN
1	A	345	GLN
1	A	385	HIS
1	A	416	GLN
1	A	434	ASN
2	I	18	GLN
2	I	22	GLN
2	I	45	ASN
2	I	70	ASN
2	I	77	ASN
2	I	78	HIS
1	C	210	ASN
1	C	216	HIS
1	C	244	ASN
1	C	345	GLN
1	C	385	HIS
1	C	416	GLN
1	C	434	ASN
2	J	18	GLN
2	J	22	GLN
2	J	45	ASN
2	J	70	ASN
2	J	78	HIS
1	E	210	ASN
1	E	216	HIS
1	E	244	ASN
1	E	345	GLN
1	E	385	HIS
1	E	416	GLN
1	E	434	ASN
2	K	18	GLN
2	K	22	GLN
2	K	45	ASN
2	K	70	ASN
2	K	78	HIS
1	G	210	ASN
1	G	216	HIS
1	G	244	ASN
1	G	345	GLN
1	G	385	HIS
1	G	416	GLN

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Mol	Chain	Res	Type
1	G	434	ASN
2	L	18	GLN
2	L	22	GLN
2	L	45	ASN
2	L	70	ASN
2	L	77	ASN
2	L	78	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	501	-	4,4,4	1.25	1 (25%)	6,6,6	0.31	0
3	PO4	A	502	-	4,4,4	1.18	1 (25%)	6,6,6	0.31	0
3	PO4	C	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.31	0
3	PO4	C	504	-	4,4,4	1.23	1 (25%)	6,6,6	0.31	0
3	PO4	E	505	-	4,4,4	1.15	1 (25%)	6,6,6	0.32	0
3	PO4	E	506	-	4,4,4	1.07	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	G	507	-	4,4,4	1.28	1 (25%)	6,6,6	0.32	0
3	PO4	G	508	-	4,4,4	1.12	1 (25%)	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	501	-	-	0/0/0/0	0/0/0/0
3	PO4	A	502	-	-	0/0/0/0	0/0/0/0
3	PO4	C	503	-	-	0/0/0/0	0/0/0/0
3	PO4	C	504	-	-	0/0/0/0	0/0/0/0
3	PO4	E	505	-	-	0/0/0/0	0/0/0/0
3	PO4	E	506	-	-	0/0/0/0	0/0/0/0
3	PO4	G	507	-	-	0/0/0/0	0/0/0/0
3	PO4	G	508	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PO4	P-O3	-2.32	1.45	1.53
3	C	503	PO4	P-O3	-2.32	1.45	1.53
3	G	507	PO4	P-O3	-2.28	1.45	1.53
3	A	502	PO4	P-O3	-2.12	1.45	1.53
3	C	504	PO4	P-O3	-2.11	1.45	1.53
3	E	505	PO4	P-O3	-2.10	1.45	1.53
3	G	508	PO4	P-O3	-2.01	1.46	1.53

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	507	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.24	40 (8%) 12 9	2, 29, 99, 100	0
1	C	445/485 (91%)	0.24	44 (9%) 9 7	2, 28, 98, 100	0
1	E	445/485 (91%)	0.42	52 (11%) 6 5	2, 31, 100, 100	0
1	G	445/485 (91%)	0.22	39 (8%) 12 10	2, 26, 98, 100	0
2	I	129/139 (92%)	0.50	16 (12%) 5 4	4, 35, 99, 100	0
2	J	129/139 (92%)	0.59	17 (13%) 4 4	2, 40, 100, 100	0
2	K	129/139 (92%)	0.63	15 (11%) 6 5	3, 41, 98, 100	0
2	L	129/139 (92%)	0.51	16 (12%) 5 4	2, 36, 100, 100	0
All	All	2296/2496 (91%)	0.34	239 (10%) 8 6	2, 31, 100, 100	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	72	VAL	12.5
1	G	72	VAL	12.5
1	E	337	LEU	10.8
1	A	74	THR	10.1
1	C	72	VAL	10.0
1	G	181	LEU	9.5
1	A	68	THR	9.3
1	A	69	TRP	9.3
1	G	73	TRP	9.3
2	K	105	ASP	9.0
1	E	181	LEU	8.8
1	E	66	THR	8.8
1	C	337	LEU	8.6
1	G	337	LEU	8.0
1	E	71	VAL	7.8
2	L	105	ASP	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	73	TRP	7.6
1	G	71	VAL	7.5
1	C	466	ASP	7.3
1	G	77	LEU	7.3
2	L	107	PRO	7.3
1	A	76	ARG	7.2
1	E	339	GLY	7.1
1	E	338	GLU	6.9
1	C	68	THR	6.8
1	C	77	LEU	6.8
1	E	82	MET	6.7
1	E	73	TRP	6.7
1	G	74	THR	6.6
1	G	66	THR	6.5
2	J	107	PRO	6.4
2	K	107	PRO	6.4
1	A	181	LEU	6.2
1	E	78	THR	5.9
1	A	337	LEU	5.8
1	E	75	ASP	5.8
2	I	105	ASP	5.8
2	I	107	PRO	5.8
1	C	78	THR	5.7
1	C	76	ARG	5.7
2	J	105	ASP	5.6
1	G	68	THR	5.5
1	C	73	TRP	5.2
2	K	1	MET	5.2
1	E	465	GLY	5.2
1	G	69	TRP	5.2
1	A	338	GLU	5.2
1	A	66	THR	5.2
1	C	181	LEU	5.2
1	G	214	PHE	5.1
1	E	80	CYS	5.0
1	E	340	ASP	5.0
2	J	108	GLY	5.0
1	G	67	ALA	5.0
1	G	334	VAL	5.0
1	C	66	THR	4.8
2	K	108	GLY	4.8
1	C	82	MET	4.8

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Mol	Chain	Res	Type	RSRZ
2	K	129	ALA	4.8
1	G	75	ASP	4.8
1	A	339	GLY	4.7
1	E	211	SER	4.7
1	E	466	ASP	4.7
1	C	334	VAL	4.6
1	G	76	ARG	4.6
1	C	69	TRP	4.6
2	I	59	ARG	4.5
1	A	72	VAL	4.5
1	C	79	ALA	4.5
1	C	75	ASP	4.5
2	K	98	PHE	4.5
1	E	214	PHE	4.4
1	E	334	VAL	4.4
1	A	466	ASP	4.4
1	C	71	VAL	4.4
1	E	77	LEU	4.3
2	K	58	LEU	4.3
2	L	108	GLY	4.2
1	E	81	ASP	4.2
2	L	98	PHE	4.2
1	E	83	TYR	4.1
1	C	180	LYS	4.0
2	J	89	HIS	4.0
1	A	70	THR	4.0
1	A	211	SER	4.0
1	A	75	ASP	4.0
1	C	445	GLU	3.8
1	A	467	ILE	3.8
1	G	78	THR	3.8
1	E	65	SER	3.7
1	C	467	ILE	3.7
1	E	95	ASN	3.7
2	I	57	ASP	3.7
1	C	182	GLY	3.7
1	C	338	GLU	3.7
2	I	101	ASN	3.7
2	J	1	MET	3.7
1	E	98	GLU	3.6
1	E	74	THR	3.6
1	A	334	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	210	ASN	3.5
1	E	50	GLY	3.5
2	I	98	PHE	3.5
1	C	465	GLY	3.5
2	K	102	ARG	3.5
2	I	129	ALA	3.5
2	J	56	PHE	3.4
1	C	83	TYR	3.4
1	A	98	GLU	3.4
1	E	70	THR	3.4
1	G	22	TYR	3.4
1	G	182	GLY	3.4
2	K	56	PHE	3.4
1	C	74	THR	3.4
1	E	69	TRP	3.3
2	J	101	ASN	3.3
1	E	467	ILE	3.3
2	L	57	ASP	3.3
1	G	338	GLU	3.3
2	J	58	LEU	3.3
1	E	22	TYR	3.3
1	G	467	ILE	3.3
2	I	88	THR	3.3
2	L	89	HIS	3.2
1	C	33	VAL	3.2
1	G	213	PRO	3.2
1	G	466	ASP	3.2
1	E	207	GLU	3.2
2	K	59	ARG	3.2
1	A	464	TRP	3.2
1	A	81	ASP	3.2
1	A	78	THR	3.2
2	J	103	PRO	3.1
1	C	207	GLU	3.1
2	J	102	ARG	3.1
1	E	464	TRP	3.1
2	L	88	THR	3.0
1	E	79	ALA	3.0
1	E	131	LYS	3.0
1	E	180	LYS	3.0
1	C	210	ASN	3.0
1	E	182	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	102	ARG	2.9
1	C	208	ASN	2.9
1	C	65	SER	2.9
2	L	129	ALA	2.9
1	A	67	ALA	2.8
1	C	84	ARG	2.8
1	C	439	ILE	2.8
1	A	31	ASP	2.8
1	C	211	SER	2.8
2	J	95	VAL	2.8
1	C	98	GLU	2.8
2	L	59	ARG	2.8
2	J	21	LYS	2.7
1	E	341	PRO	2.7
1	A	65	SER	2.7
2	K	57	ASP	2.7
1	G	82	MET	2.7
1	A	22	TYR	2.7
1	G	98	GLU	2.7
2	I	108	GLY	2.7
2	L	60	ASP	2.6
1	C	64	SER	2.6
1	C	80	CYS	2.6
2	K	103	PRO	2.6
1	G	207	GLU	2.6
1	A	458	ARG	2.6
1	C	22	TYR	2.6
1	E	342	LEU	2.6
1	A	333	ALA	2.6
1	E	67	ALA	2.6
1	G	210	ASN	2.5
1	G	211	SER	2.5
2	L	58	LEU	2.5
1	A	80	CYS	2.5
2	I	89	HIS	2.5
1	A	49	ASP	2.5
1	G	206	ASP	2.5
2	K	95	VAL	2.5
1	A	180	LYS	2.4
1	E	26	GLY	2.4
2	K	90	THR	2.4
2	J	106	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	278	CYS	2.4
2	J	88	THR	2.4
1	G	49	ASP	2.4
1	E	33	VAL	2.4
2	L	102	ARG	2.4
1	A	414	GLY	2.4
1	A	71	VAL	2.4
1	A	207	GLU	2.3
1	C	336	LYS	2.3
1	C	70	THR	2.3
1	G	452	ARG	2.3
2	I	103	PRO	2.3
1	C	95	ASN	2.3
1	G	464	TRP	2.3
1	E	426	LEU	2.3
1	A	82	MET	2.3
1	C	464	TRP	2.3
1	G	83	TYR	2.3
2	I	87	SER	2.3
2	L	90	THR	2.3
1	E	52	ASP	2.2
1	G	131	LYS	2.2
1	G	180	LYS	2.2
1	C	456	PRO	2.2
1	E	28	TRP	2.2
1	C	214	PHE	2.2
2	J	90	THR	2.2
1	E	441	ASN	2.2
2	J	44	ARG	2.2
1	A	64	SER	2.2
2	I	77	ASN	2.2
1	G	439	ILE	2.1
1	E	336	LYS	2.1
1	A	214	PHE	2.1
1	E	357	GLN	2.1
1	E	68	THR	2.1
1	E	210	ASN	2.1
2	I	119	ARG	2.1
2	L	44	ARG	2.1
1	C	67	ALA	2.1
1	G	332	THR	2.1
1	G	445	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	129	ALA	2.1
1	A	77	LEU	2.1
2	L	95	VAL	2.1
1	A	209	ILE	2.1
1	E	25	MET	2.1
1	E	456	PRO	2.1
2	L	1	MET	2.1
1	G	70	THR	2.0
1	C	49	ASP	2.0
2	K	77	ASN	2.0
2	I	1	MET	2.0
1	G	336	LYS	2.0
1	A	332	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	502	5/5	0.97	0.25	0.30	18,23,40,42	0
3	PO4	C	503	5/5	0.95	0.22	0.12	18,23,40,42	0
3	PO4	E	506	5/5	0.93	0.33	0.09	18,23,40,42	0
3	PO4	C	504	5/5	0.94	0.25	-0.04	18,23,40,42	0
3	PO4	G	507	5/5	0.95	0.18	-0.12	18,23,40,42	0
3	PO4	A	501	5/5	0.95	0.22	-0.23	18,23,40,42	0
3	PO4	G	508	5/5	0.92	0.25	-0.24	18,23,40,42	0
3	PO4	E	505	5/5	0.97	0.20	-0.28	18,23,40,42	0

6.5 Other polymers

There are no such residues in this entry.