



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 04:05 PM UTC

PDB ID : 8EU4 / pdb_00008eu4
Title : Escherichia coli pyruvate kinase A301S
Authors : Donovan, K.A.; Coombes, D.; Dobson, R.C.J.; Cooper, T.F.
Deposited on : 2022-10-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

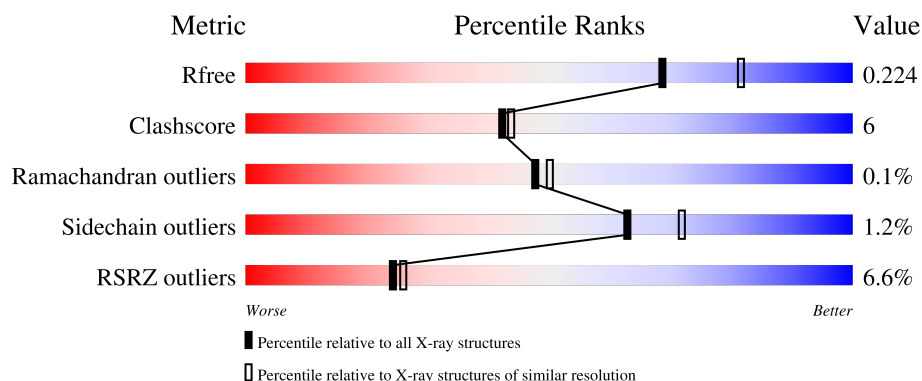
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



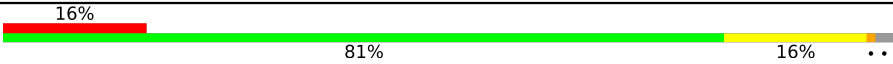
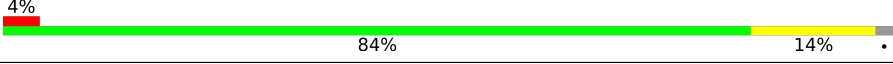
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	470	15% 86% 12% .
1	B	470	2% 88% 10% ..
1	C	470	5% 86% 12% .
1	D	470	3% 86% 12% ..
1	E	470	3% 84% 13% .

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Mol	Chain	Length	Quality of chain
1	F	470	
1	G	470	
1	H	470	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 57299 atoms, of which 28463 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	462	Total	C	H	N	O	S	0	0	0
			7003	2155	3542	600	682	24			
1	E	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	D	462	Total	C	H	N	O	S	0	0	0
			7030	2161	3562	601	682	24			
1	G	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	B	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	F	461	Total	C	H	N	O	S	0	0	0
			6991	2152	3538	596	681	24			
1	H	462	Total	C	H	N	O	S	0	0	0
			7030	2161	3562	601	682	24			
1	C	462	Total	C	H	N	O	S	0	0	0
			6998	2155	3540	597	682	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	SER	ALA	engineered mutation	UNP A0A0A0G552
E	301	SER	ALA	engineered mutation	UNP A0A0A0G552
D	301	SER	ALA	engineered mutation	UNP A0A0A0G552
G	301	SER	ALA	engineered mutation	UNP A0A0A0G552
B	301	SER	ALA	engineered mutation	UNP A0A0A0G552
F	301	SER	ALA	engineered mutation	UNP A0A0A0G552
H	301	SER	ALA	engineered mutation	UNP A0A0A0G552
C	301	SER	ALA	engineered mutation	UNP A0A0A0G552

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	E	153	Total	O	0	0
			153	153		
3	D	146	Total	O	0	0
			146	146		
3	G	157	Total	O	0	0
			157	157		

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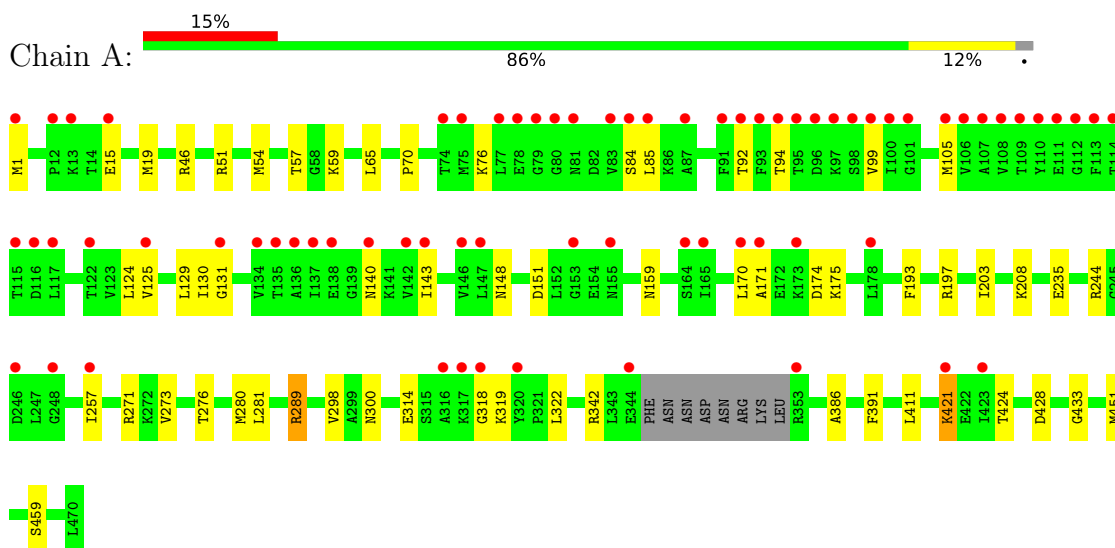
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	169	Total 169	O 169	0	0
3	F	103	Total 103	O 103	0	0
3	H	114	Total 114	O 114	0	0
3	C	120	Total 120	O 120	0	0

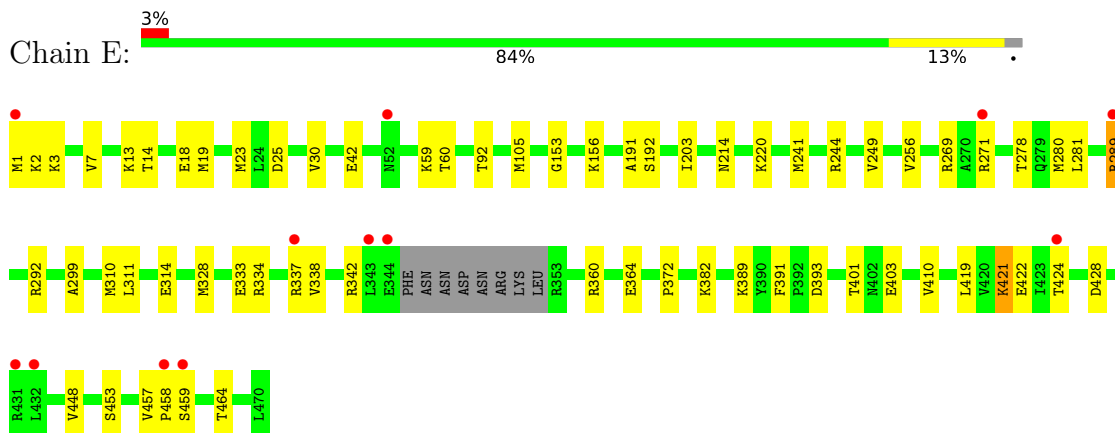
3 Residue-property plots

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

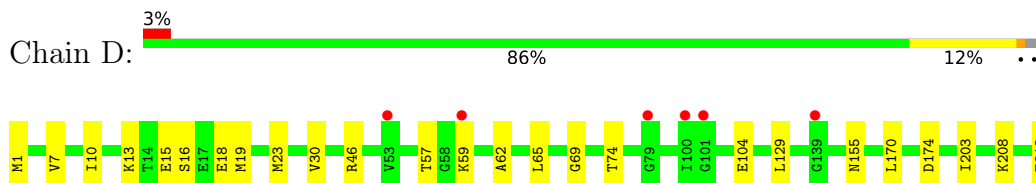
• Molecule 1: Pyruvate kinase

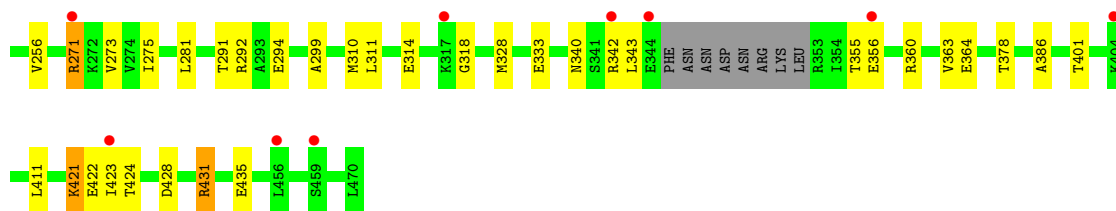


• Molecule 1: Pyruvate kinase

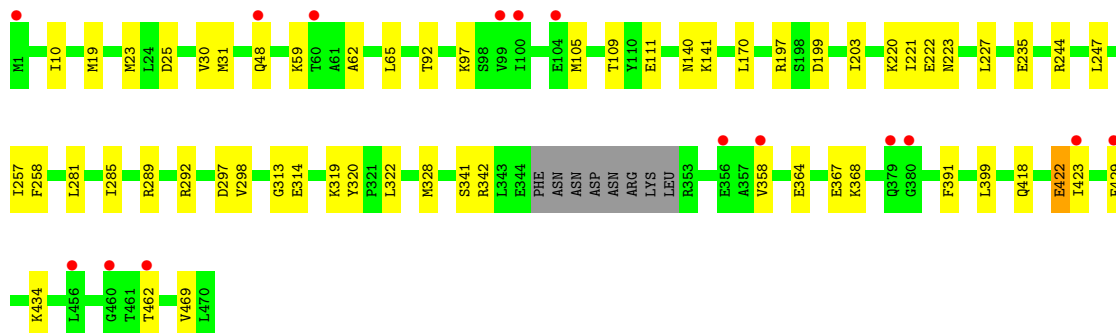
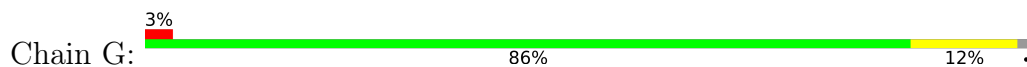


• Molecule 1: Pyruvate kinase

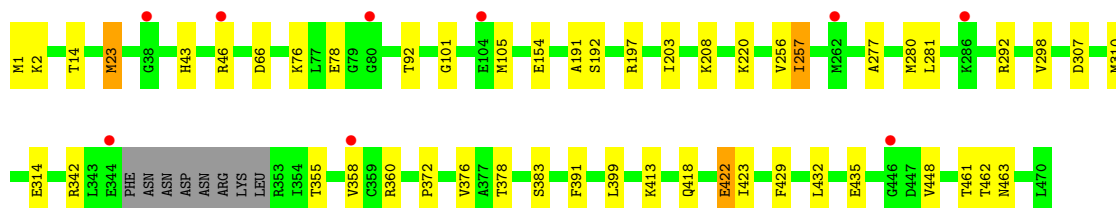
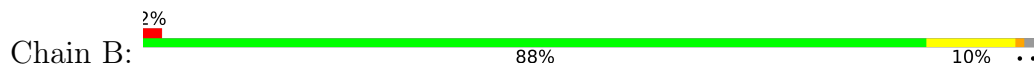




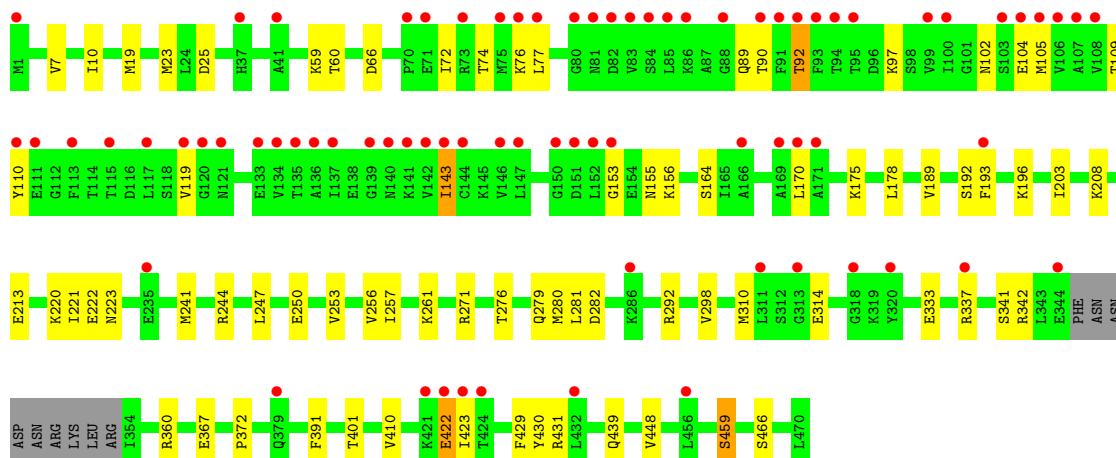
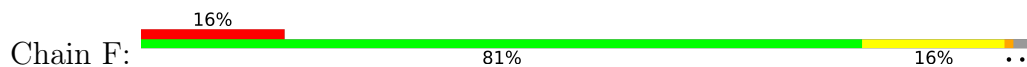
● Molecule 1: Pyruvate kinase



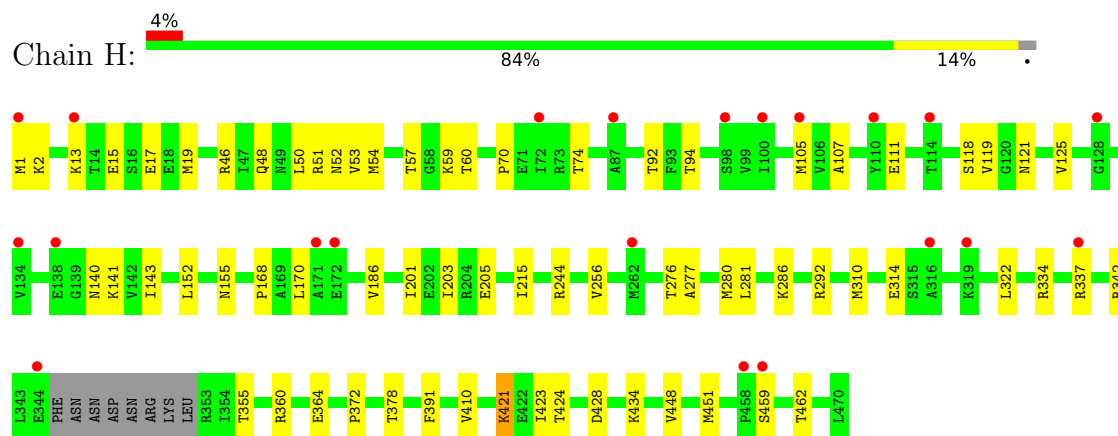
● Molecule 1: Pyruvate kinase



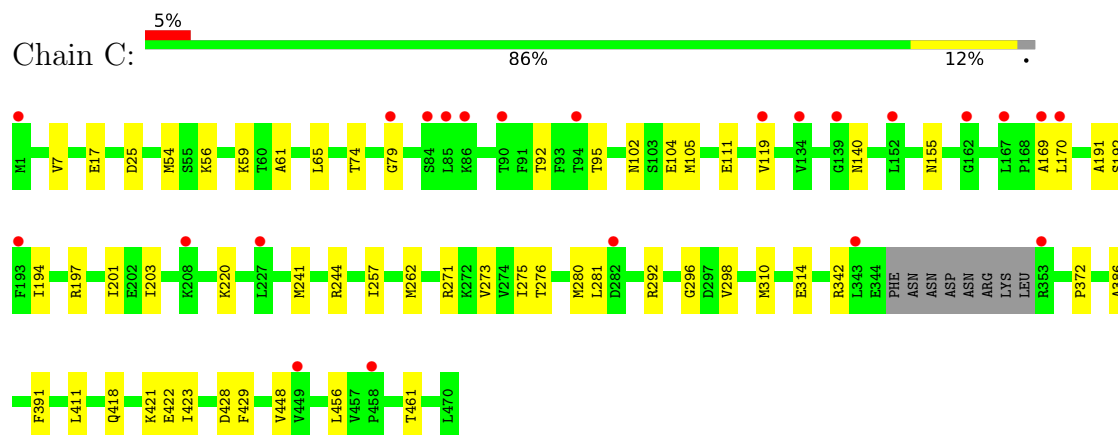
● Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.33Å 74.47Å 240.83Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	48.17 – 2.10 48.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.17-2.10) 99.9 (48.17-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.224 0.201 , 0.224	Depositor DCC
R_{free} test set	13639 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.080 for h,-k,-l	Depositor
Outliers	9 of 267878 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	57299	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/3495	0.46	0/4713
1	B	0.25	0/3508	0.48	0/4728
1	C	0.20	0/3492	0.43	0/4710
1	D	0.25	0/3502	0.49	0/4721
1	E	0.26	0/3508	0.48	0/4728
1	F	0.34	1/3487 (0.0%)	0.52	1/4703 (0.0%)
1	G	0.24	0/3508	0.47	0/4728
1	H	0.22	0/3502	0.45	0/4721
All	All	0.25	1/28002 (0.0%)	0.47	1/37752 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	ILE	CG1-CD1	-10.57	1.10	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	THR	OG1-CB-CG2	7.88	125.05	109.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	271	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3461	3542	3542	45	0
1	B	3474	3573	3573	37	0
1	C	3458	3540	3540	40	1
1	D	3468	3562	3562	49	0
1	E	3474	3573	3573	52	1
1	F	3453	3538	3538	57	0
1	G	3474	3573	3573	45	0
1	H	3468	3562	3562	50	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	1	0
3	A	104	0	0	1	0
3	B	169	0	0	2	0
3	C	120	0	0	0	0
3	D	146	0	0	1	0
3	E	153	0	0	1	0
3	F	103	0	0	3	0
3	G	157	0	0	3	0
3	H	114	0	0	1	0
All	All	28836	28463	28463	354	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (354) 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:F:92:THR:HG21	1:F:105:MET:HE2	1.47	0.94
1:B:277:ALA:HB1	1:B:310:MET:HE2	1.52	0.90
1:H:277:ALA:HB1	1:H:310:MET:HE2	1.54	0.89
1:F:175:LYS:NZ	3:F:601:HOH:O	2.03	0.83
1:D:15:GLU:OE1	1:D:46:ARG:NH1	2.12	0.82
1:C:7:VAL:HG11	1:C:310:MET:HE2	1.64	0.80
1:C:241:MET:HE2	1:C:310:MET:HE1	1.63	0.79
1:D:57:THR:HG21	1:D:59:LYS:HE3	1.65	0.78
1:F:72:ILE:HD12	1:F:110:TYR:HB2	1.64	0.77
1:E:14:THR:HA	1:E:19:MET:HG2	1.66	0.77
1:A:257:ILE:HD12	1:A:257:ILE:H	1.49	0.76
1:D:241:MET:HE2	1:D:310:MET:HE1	1.66	0.76
1:G:25:ASP:OD1	1:G:59:LYS:NZ	2.19	0.75
1:A:19:MET:HE1	1:A:322:LEU:HG	1.67	0.74
1:F:92:THR:CG2	1:F:105:MET:HE2	2.18	0.73
1:B:192:SER:HA	1:B:220:LYS:HD2	1.71	0.73
1:E:244:ARG:NH2	1:E:280:MET:SD	2.62	0.72
1:E:401:THR:HG21	1:E:422:GLU:HA	1.71	0.72
1:F:423:ILE:HG21	1:F:429:PHE:HB2	1.71	0.72
1:E:334:ARG:HD2	1:E:337:ARG:HE	1.54	0.72
1:A:257:ILE:HG12	1:C:296:GLY:HA2	1.70	0.71
1:C:25:ASP:OD1	1:C:59:LYS:NZ	2.23	0.71
1:A:99:VAL:HG11	1:A:105:MET:HE3	1.72	0.71
1:D:241:MET:CE	1:D:310:MET:HE1	2.20	0.71
1:G:227:LEU:HD21	1:G:247:LEU:HD21	1.71	0.70
1:H:170:LEU:HD21	1:H:203:ILE:CD1	2.22	0.70
1:E:60:THR:HG22	1:E:410:VAL:HG21	1.73	0.70
1:D:291:THR:HG23	1:D:294:GLU:H	1.57	0.70
1:H:17:GLU:HG2	1:H:53:VAL:HG23	1.74	0.70
1:F:241:MET:HE2	1:F:310:MET:HE1	1.75	0.69
1:A:271:ARG:HG2	1:A:386:ALA:HA	1.75	0.68
1:C:197:ARG:CZ	1:C:201:ILE:HD11	2.23	0.68
1:H:92:THR:HG23	1:H:143:ILE:HD13	1.75	0.68
1:D:271:ARG:CZ	1:D:356:GLU:HG2	2.24	0.67
1:F:333:GLU:OE1	1:F:337:ARG:NH2	2.25	0.67
1:C:95:THR:HG22	1:C:140:ASN:HB2	1.77	0.66
1:D:340:ASN:O	1:D:342:ARG:NH1	2.29	0.66
1:F:92:THR:HB	1:F:105:MET:HG3	1.78	0.65
1:B:280:MET:HE3	1:B:298:VAL:HG22	1.78	0.65
1:H:50:LEU:HG	1:H:54:MET:HE2	1.79	0.65
1:F:25:ASP:OD1	1:F:59:LYS:NZ	2.30	0.65
1:D:271:ARG:HH12	1:D:355:THR:HG22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG2	1:B:2:LYS:H	1.63	0.64
1:D:16:SER:OG	1:D:18:GLU:HG2	1.97	0.64
1:D:360:ARG:NH2	1:D:364:GLU:OE1	2.25	0.63
1:F:208:LYS:HG3	1:F:213:GLU:HB3	1.78	0.63
1:E:292:ARG:HD2	1:G:244:ARG:HB3	1.79	0.63
1:F:256:VAL:HG11	1:H:292:ARG:HD2	1.81	0.63
1:B:277:ALA:HB1	1:B:310:MET:CE	2.27	0.62
1:H:186:VAL:O	1:H:215:ILE:HD12	1.99	0.62
1:C:241:MET:CE	1:C:310:MET:HE1	2.30	0.62
1:E:360:ARG:NH2	1:E:364:GLU:OE1	2.24	0.61
1:E:453:SER:O	1:E:464:THR:HG22	2.01	0.60
1:E:342:ARG:HD2	1:E:391:PHE:CD1	2.36	0.60
1:G:111:GLU:OE1	3:G:601:HOH:O	2.17	0.60
1:G:285:ILE:HD11	1:G:313:GLY:C	2.27	0.60
1:F:342:ARG:HD2	1:F:391:PHE:CD1	2.38	0.59
1:F:241:MET:CE	1:F:310:MET:HE1	2.32	0.59
1:H:92:THR:O	1:H:105:MET:HG3	2.03	0.59
1:E:25:ASP:OD1	1:E:59:LYS:NZ	2.36	0.59
1:F:292:ARG:HG3	1:H:256:VAL:HG11	1.85	0.59
1:H:280:MET:HE2	1:H:280:MET:HA	1.85	0.58
1:B:342:ARG:HD2	1:B:391:PHE:CD1	2.38	0.58
1:B:78:GLU:HG3	1:B:101:GLY:O	2.04	0.58
1:F:153:GLY:H	1:F:156:LYS:HZ2	1.52	0.58
1:H:424:THR:HG23	1:H:428:ASP:OD2	2.03	0.58
1:C:342:ARG:HD2	1:C:391:PHE:CD1	2.39	0.58
1:E:292:ARG:NH2	1:G:297:ASP:OD2	2.36	0.58
1:A:342:ARG:HD2	1:A:391:PHE:CD1	2.40	0.57
1:E:337:ARG:NH2	3:E:601:HOH:O	2.26	0.57
1:A:280:MET:HE3	1:A:298:VAL:HG22	1.87	0.57
1:A:170:LEU:HD11	1:A:203:ILE:HD13	1.85	0.57
1:A:85:LEU:N	1:A:85:LEU:HD12	2.20	0.57
1:G:342:ARG:HD2	1:G:391:PHE:CD1	2.40	0.57
1:D:275:ILE:HG21	1:D:310:MET:HE3	1.87	0.56
1:E:241:MET:CE	1:E:310:MET:HE1	2.36	0.56
1:G:223:ASN:O	1:G:227:LEU:HD23	2.05	0.56
1:F:271:ARG:NE	3:F:602:HOH:O	2.38	0.56
1:H:17:GLU:HG2	1:H:53:VAL:CG2	2.37	0.55
1:C:194:ILE:HD12	1:C:194:ILE:N	2.20	0.55
1:B:197:ARG:NH1	3:B:602:HOH:O	2.39	0.55
1:F:7:VAL:HG11	1:F:310:MET:HE2	1.89	0.55
1:F:193:PHE:N	1:F:222:GLU:OE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ARG:NH2	1:D:386:ALA:HB1	2.22	0.55
1:C:273:VAL:HG21	1:C:411:LEU:HG	1.89	0.55
1:G:170:LEU:HD21	1:G:203:ILE:CD1	2.36	0.55
1:E:153:GLY:HA3	1:E:156:LYS:HZ2	1.72	0.55
1:H:421:LYS:HD2	1:H:421:LYS:N	2.22	0.55
1:C:275:ILE:HG21	1:C:310:MET:HE3	1.88	0.54
1:A:57:THR:HB	1:A:59:LYS:HE2	1.89	0.54
1:E:281:LEU:O	1:E:314:GLU:HG2	2.07	0.54
1:E:403:GLU:HA	1:E:419:LEU:HD21	1.89	0.54
1:E:299:ALA:HB3	1:G:257:ILE:HD13	1.87	0.54
1:C:280:MET:HE3	1:C:298:VAL:HG22	1.88	0.54
1:C:244:ARG:HD2	1:C:276:THR:HG23	1.89	0.54
1:A:459:SER:O	2:A:501:SO4:O4	2.25	0.54
1:F:341:SER:OG	1:F:367:GLU:OE2	2.09	0.54
1:E:459:SER:O	2:E:501:SO4:O4	2.25	0.54
1:D:421:LYS:H	1:D:421:LYS:HD3	1.72	0.54
1:A:1:MET:HG2	1:A:1:MET:O	2.08	0.53
1:C:191:ALA:CB	1:C:203:ILE:HD13	2.38	0.53
1:G:140:ASN:OD1	1:G:141:LYS:HD2	2.07	0.53
1:G:197:ARG:NH2	1:G:235:GLU:HB3	2.23	0.53
1:E:334:ARG:CZ	1:E:337:ARG:NH2	2.72	0.53
1:H:342:ARG:HD2	1:H:391:PHE:CD1	2.42	0.53
1:F:76:LYS:O	1:F:77:LEU:HD23	2.08	0.53
1:A:15:GLU:HB2	1:A:46:ARG:HG2	1.91	0.53
1:D:170:LEU:HD21	1:D:203:ILE:HG12	1.90	0.53
1:B:76:LYS:HA	1:B:154:GLU:CG	2.39	0.53
1:F:92:THR:HB	1:F:105:MET:CG	2.39	0.53
1:A:51:ARG:HA	1:A:54:MET:HE3	1.90	0.53
1:H:140:ASN:OD1	1:H:141:LYS:HD2	2.08	0.53
1:C:423:ILE:HG23	1:C:428:ASP:OD2	2.08	0.53
1:A:19:MET:HE1	1:A:322:LEU:CG	2.38	0.53
1:A:170:LEU:CD2	1:A:174:ASP:HB3	2.39	0.53
1:H:170:LEU:HD21	1:H:203:ILE:HD12	1.90	0.53
1:E:7:VAL:HG11	1:E:310:MET:HE2	1.91	0.53
1:D:299:ALA:HB3	1:B:257:ILE:HD12	1.91	0.53
1:B:432:LEU:O	1:B:435:GLU:HG2	2.09	0.53
1:H:186:VAL:O	1:H:215:ILE:CD1	2.58	0.52
1:D:378:THR:OG1	2:D:501:SO4:O1	2.26	0.52
1:F:223:ASN:HB2	1:F:250:GLU:OE1	2.10	0.52
1:B:14:THR:HB	1:B:23:MET:HE1	1.90	0.52
1:D:343:LEU:HD21	1:D:363:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:ARG:HG3	1:G:258:PHE:CE2	2.45	0.52
1:G:281:LEU:O	1:G:314:GLU:HG2	2.10	0.52
1:F:97:LYS:HE3	1:F:109:THR:HA	1.91	0.52
1:H:92:THR:CG2	1:H:143:ILE:HD13	2.38	0.51
1:H:360:ARG:NH2	1:H:364:GLU:OE1	2.36	0.51
1:G:170:LEU:HD21	1:G:203:ILE:HD12	1.91	0.51
1:E:271:ARG:HH22	1:E:382:LYS:HB3	1.74	0.51
1:D:291:THR:CG2	1:D:294:GLU:HG3	2.40	0.51
1:H:51:ARG:HA	1:H:54:MET:HE3	1.93	0.51
1:F:292:ARG:CD	1:H:256:VAL:HG11	2.41	0.51
1:G:221:ILE:CG2	1:G:227:LEU:HD22	2.40	0.51
1:A:244:ARG:HB3	1:C:292:ARG:HD2	1.93	0.51
1:F:60:THR:HG22	1:F:410:VAL:HG21	1.93	0.51
1:C:191:ALA:O	1:C:194:ILE:CD1	2.58	0.51
1:F:281:LEU:O	1:F:314:GLU:HG2	2.11	0.51
1:B:281:LEU:O	1:B:314:GLU:HG2	2.11	0.50
1:H:19:MET:HE1	1:H:322:LEU:HG	1.94	0.50
1:G:342:ARG:NE	3:G:602:HOH:O	2.40	0.50
1:D:273:VAL:HG21	1:D:411:LEU:HG	1.93	0.50
1:E:241:MET:HE2	1:E:310:MET:HE1	1.92	0.50
1:E:334:ARG:O	1:E:337:ARG:HG2	2.12	0.50
1:G:30:VAL:HG22	1:G:62:ALA:HB3	1.94	0.50
1:A:170:LEU:CD1	1:A:203:ILE:HD13	2.42	0.50
1:C:17:GLU:OE1	1:C:56:LYS:NZ	2.23	0.50
1:C:271:ARG:HG2	1:C:386:ALA:HA	1.93	0.50
1:D:256:VAL:HG11	1:B:292:ARG:HG3	1.93	0.49
1:F:292:ARG:CG	1:H:256:VAL:HG11	2.42	0.49
1:E:337:ARG:HG3	1:E:338:VAL:HG13	1.94	0.49
1:F:72:ILE:HD12	1:F:110:TYR:CB	2.37	0.49
1:F:401:THR:CG2	1:F:422:GLU:HA	2.42	0.49
1:E:334:ARG:HD2	1:E:337:ARG:NE	2.26	0.49
1:C:95:THR:OG1	1:C:111:GLU:HA	2.13	0.49
1:H:280:MET:HG3	1:H:310:MET:O	2.12	0.49
1:H:57:THR:HB	1:H:59:LYS:HE2	1.94	0.49
1:G:399:LEU:HD23	1:G:418:GLN:HB3	1.93	0.49
1:B:422:GLU:C	1:B:423:ILE:HG13	2.38	0.49
1:G:341:SER:HB3	1:G:367:GLU:OE2	2.11	0.49
1:H:48:GLN:NE2	1:H:52:ASN:OD1	2.42	0.49
1:A:125:VAL:CG1	1:A:130:ILE:HB	2.43	0.49
1:A:197:ARG:NH1	1:A:235:GLU:OE1	2.46	0.49
1:D:18:GLU:HG3	1:D:19:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:THR:HG22	1:H:410:VAL:HG21	1.95	0.49
1:E:424:THR:HG23	1:E:428:ASP:OD2	2.12	0.49
1:F:92:THR:CB	1:F:105:MET:HE2	2.42	0.49
1:C:102:ASN:OD1	1:C:104:GLU:HG2	2.12	0.49
1:D:424:THR:HG23	1:D:428:ASP:OD2	2.13	0.49
1:G:423:ILE:HG21	1:G:429:PHE:HB2	1.95	0.48
1:C:169:ALA:C	1:C:170:LEU:HD12	2.38	0.48
1:A:171:ALA:O	1:A:175:LYS:HG3	2.13	0.48
1:F:256:VAL:HG11	1:H:292:ARG:CD	2.43	0.48
1:F:10:ILE:CD1	1:F:23:MET:HE2	2.43	0.48
1:D:281:LEU:O	1:D:314:GLU:HG2	2.14	0.48
1:A:300:ASN:HD21	1:C:257:ILE:HD11	1.78	0.48
1:E:3:LYS:NZ	1:E:393:ASP:O	2.38	0.48
1:G:319:LYS:HE3	1:G:320:TYR:CZ	2.49	0.47
1:G:364:GLU:HG2	1:G:368:LYS:HE3	1.95	0.47
1:H:244:ARG:NH2	1:H:280:MET:HE3	2.29	0.47
1:E:153:GLY:HA3	1:E:156:LYS:NZ	2.29	0.47
1:F:430:TYR:OH	1:F:466:SER:OG	2.23	0.47
1:H:281:LEU:O	1:H:314:GLU:HG2	2.14	0.47
1:B:66:ASP:OD1	1:B:220:LYS:HE3	2.15	0.47
1:A:257:ILE:CG1	1:C:296:GLY:HA2	2.42	0.47
1:E:249:VAL:HG12	1:E:249:VAL:O	2.14	0.47
1:G:422:GLU:C	1:G:423:ILE:HG13	2.39	0.47
1:F:253:VAL:HA	3:F:606:HOH:O	2.15	0.47
1:H:244:ARG:CZ	1:H:280:MET:HE3	2.44	0.47
1:D:421:LYS:H	1:D:421:LYS:CD	2.28	0.47
1:C:95:THR:CG2	1:C:140:ASN:HB2	2.43	0.47
1:F:279:GLN:HA	1:F:282:ASP:OD2	2.15	0.47
1:G:341:SER:CB	1:G:367:GLU:OE2	2.63	0.47
1:B:423:ILE:HG21	1:B:429:PHE:HB2	1.97	0.47
1:D:291:THR:HG22	1:D:294:GLU:CD	2.40	0.47
1:G:434:LYS:NZ	1:G:469:VAL:O	2.48	0.47
1:H:423:ILE:HD13	3:H:666:HOH:O	2.15	0.47
1:A:257:ILE:H	1:A:257:ILE:CD1	2.19	0.46
1:D:18:GLU:CG	1:D:19:MET:N	2.78	0.46
1:D:422:GLU:CD	1:D:423:ILE:H	2.23	0.46
1:E:457:VAL:HB	1:E:458:PRO:HD2	1.98	0.46
1:D:57:THR:HG22	1:D:57:THR:O	2.15	0.46
1:D:401:THR:CG2	1:D:422:GLU:HA	2.45	0.46
1:D:292:ARG:CG	1:B:256:VAL:HG11	2.46	0.46
1:H:334:ARG:O	1:H:337:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ARG:HA	1:E:389:LYS:NZ	2.31	0.46
1:D:10:ILE:HG22	1:D:46:ARG:HD3	1.98	0.46
1:G:220:LYS:HD2	1:G:222:GLU:OE2	2.15	0.46
1:G:19:MET:O	1:G:23:MET:HG2	2.15	0.46
1:A:421:LYS:HE3	1:A:421:LYS:HA	1.97	0.46
1:C:170:LEU:HD12	1:C:170:LEU:N	2.31	0.46
1:E:2:LYS:HB3	1:E:333:GLU:HG3	1.98	0.46
1:E:191:ALA:HB1	1:E:203:ILE:HD13	1.97	0.46
1:D:57:THR:CG2	1:D:59:LYS:HG3	2.46	0.46
1:F:192:SER:HA	1:F:220:LYS:HD2	1.97	0.46
1:A:131:GLY:H	1:A:148:ASN:HD21	1.64	0.46
1:A:424:THR:HG23	1:A:428:ASP:OD2	2.16	0.46
1:B:277:ALA:CB	1:B:310:MET:HE2	2.35	0.46
1:F:220:LYS:HD3	1:F:222:GLU:OE2	2.16	0.45
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.97	0.45
1:C:281:LEU:O	1:C:314:GLU:HG2	2.16	0.45
1:E:191:ALA:CB	1:E:203:ILE:HD13	2.47	0.45
1:F:89:GLN:HG2	1:F:90:THR:N	2.32	0.45
1:D:401:THR:HG22	1:D:422:GLU:HA	1.97	0.45
1:F:102:ASN:CG	1:F:104:GLU:OE1	2.59	0.45
1:E:60:THR:HG22	1:E:410:VAL:CG2	2.43	0.45
1:B:208:LYS:HD2	3:B:743:HOH:O	2.16	0.45
1:H:15:GLU:HB2	1:H:46:ARG:HG2	1.98	0.45
1:G:422:GLU:O	1:G:423:ILE:HG13	2.15	0.45
1:F:170:LEU:HD21	1:F:203:ILE:HD12	1.99	0.45
1:F:280:MET:HE3	1:F:298:VAL:HG22	1.99	0.45
1:B:191:ALA:CB	1:B:203:ILE:HD13	2.47	0.45
1:D:291:THR:HG22	1:D:294:GLU:OE1	2.17	0.45
1:A:433:GLY:HA3	1:A:451:MET:CE	2.47	0.44
1:C:169:ALA:CB	1:C:170:LEU:HD12	2.46	0.44
1:D:19:MET:O	1:D:23:MET:HG2	2.16	0.44
1:D:271:ARG:HH12	1:D:355:THR:CG2	2.27	0.44
1:A:281:LEU:O	1:A:314:GLU:HG2	2.17	0.44
1:G:298:VAL:HG11	1:G:328:MET:SD	2.58	0.44
1:B:378:THR:HB	1:B:383:SER:HG	1.82	0.44
1:H:125:VAL:HG11	1:H:152:LEU:HD13	1.99	0.44
1:D:69:GLY:HA2	1:D:174:ASP:OD2	2.18	0.44
1:F:430:TYR:HH	1:F:466:SER:HG	1.52	0.44
1:H:70:PRO:HG3	1:H:168:PRO:O	2.18	0.44
1:H:277:ALA:CB	1:H:310:MET:HE2	2.37	0.44
1:E:421:LYS:CD	1:E:421:LYS:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:VAL:HG21	1:B:463:ASN:HA	2.00	0.44
1:B:372:PRO:HD2	1:B:448:VAL:O	2.18	0.44
1:A:94:THR:HA	1:A:140:ASN:O	2.18	0.44
1:A:273:VAL:HG21	1:A:411:LEU:HG	2.00	0.44
1:G:199:ASP:O	1:G:203:ILE:HG12	2.18	0.44
1:F:19:MET:O	1:F:23:MET:HG2	2.18	0.44
1:C:422:GLU:HG2	1:C:423:ILE:N	2.33	0.44
1:A:170:LEU:HD11	1:A:203:ILE:CD1	2.48	0.43
1:D:333:GLU:HG3	3:D:698:HOH:O	2.18	0.43
1:H:74:THR:O	1:H:155:ASN:HA	2.18	0.43
1:F:257:ILE:HG12	1:F:261:LYS:HE2	2.00	0.43
1:E:7:VAL:HG22	1:E:30:VAL:HB	2.01	0.43
1:E:401:THR:CG2	1:E:422:GLU:HA	2.45	0.43
1:F:143:ILE:HA	1:F:143:ILE:HD13	1.83	0.43
1:F:244:ARG:HD2	1:F:276:THR:HG23	1.99	0.43
1:A:244:ARG:HD2	1:A:276:THR:HG23	2.01	0.43
1:D:74:THR:O	1:D:155:ASN:HA	2.19	0.43
1:G:227:LEU:HD21	1:G:247:LEU:CD2	2.45	0.43
1:E:334:ARG:HG3	1:G:258:PHE:HE2	1.83	0.43
1:A:257:ILE:HD12	1:A:257:ILE:N	2.25	0.43
1:E:19:MET:O	1:E:23:MET:HG2	2.18	0.43
1:E:311:LEU:HD21	1:E:328:MET:HE2	2.01	0.43
1:E:372:PRO:HD2	1:E:448:VAL:O	2.19	0.43
1:G:92:THR:O	1:G:105:MET:HA	2.18	0.43
1:F:221:ILE:HG22	1:F:247:LEU:HD11	2.01	0.43
1:A:85:LEU:N	1:A:85:LEU:CD1	2.81	0.43
1:A:318:GLY:HA3	3:A:607:HOH:O	2.17	0.43
1:G:97:LYS:HE3	1:G:109:THR:HA	2.01	0.43
1:C:456:LEU:HD12	1:C:456:LEU:N	2.34	0.43
1:E:1:MET:HG3	1:E:333:GLU:HG2	2.01	0.42
1:D:208:LYS:HD3	1:D:213:GLU:HB3	2.01	0.42
1:H:57:THR:CB	1:H:59:LYS:HE2	2.49	0.42
1:H:378:THR:OG1	2:H:501:SO4:O3	2.36	0.42
1:A:124:LEU:HB2	1:A:159:ASN:HB2	2.01	0.42
1:D:13:LYS:CD	1:D:318:GLY:O	2.67	0.42
1:G:10:ILE:HG12	1:G:31:MET:HG3	2.01	0.42
1:G:319:LYS:HE3	1:G:320:TYR:OH	2.19	0.42
1:E:92:THR:O	1:E:105:MET:HA	2.19	0.42
1:D:256:VAL:HG11	1:B:292:ARG:CG	2.49	0.42
1:F:92:THR:HG23	1:F:143:ILE:HD13	2.01	0.42
1:C:192:SER:HA	1:C:220:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HG2	1:A:193:PHE:CD2	2.55	0.42
1:E:271:ARG:NH2	1:E:382:LYS:HB3	2.34	0.42
1:D:7:VAL:HG11	1:D:310:MET:HE2	2.02	0.42
1:H:201:ILE:O	1:H:205:GLU:HG3	2.19	0.42
1:C:191:ALA:CB	1:C:194:ILE:HD11	2.50	0.42
1:G:285:ILE:CD1	1:G:313:GLY:C	2.91	0.42
1:F:241:MET:HE2	1:F:310:MET:CE	2.46	0.42
1:E:289:ARG:HD2	1:E:289:ARG:H	1.85	0.42
1:E:244:ARG:NH2	1:E:278:THR:O	2.45	0.42
1:F:66:ASP:OD1	1:F:220:LYS:NZ	2.48	0.42
1:D:30:VAL:HG22	1:D:62:ALA:HB3	2.02	0.42
1:B:23:MET:HE2	1:B:23:MET:HB2	1.85	0.42
1:D:1:MET:HE3	1:D:333:GLU:OE1	2.20	0.42
1:B:422:GLU:O	1:B:423:ILE:HG13	2.19	0.42
1:B:43:HIS:CE1	1:B:46:ARG:NH1	2.87	0.41
1:F:164:SER:OG	1:F:196:LYS:NZ	2.50	0.41
1:F:92:THR:O	1:F:105:MET:HA	2.20	0.41
1:C:92:THR:O	1:C:105:MET:HA	2.19	0.41
1:A:57:THR:CB	1:A:59:LYS:HE2	2.49	0.41
1:A:65:LEU:HD23	1:A:65:LEU:C	2.45	0.41
1:E:256:VAL:HG11	1:G:292:ARG:CG	2.50	0.41
1:E:292:ARG:CD	1:G:244:ARG:HB3	2.47	0.41
1:B:76:LYS:HA	1:B:154:GLU:HG3	2.02	0.41
1:B:376:VAL:CG1	1:B:383:SER:OG	2.68	0.41
1:A:84:SER:OG	1:A:151:ASP:OD1	2.28	0.41
1:H:372:PRO:HD2	1:H:448:VAL:O	2.20	0.41
1:B:399:LEU:HD23	1:B:418:GLN:HB3	2.01	0.41
1:A:92:THR:O	1:A:105:MET:HA	2.21	0.41
1:G:19:MET:HE1	1:G:322:LEU:HG	2.02	0.41
1:G:358:VAL:HG21	1:G:462:THR:O	2.20	0.41
1:B:92:THR:O	1:B:105:MET:HA	2.21	0.41
1:F:178:LEU:HD21	1:F:189:VAL:HG11	2.03	0.41
1:F:372:PRO:HD2	1:F:448:VAL:O	2.21	0.41
1:H:434:LYS:N	1:H:451:MET:HE1	2.36	0.41
1:A:289:ARG:H	1:A:289:ARG:HD3	1.85	0.41
1:B:355:THR:HA	1:B:462:THR:O	2.20	0.41
1:F:89:GLN:HG2	1:F:90:THR:O	2.21	0.41
1:F:292:ARG:HD2	1:H:256:VAL:HG11	2.02	0.41
1:H:118:SER:N	1:H:121:ASN:OD1	2.48	0.41
1:H:244:ARG:HD2	1:H:276:THR:HG23	2.02	0.41
1:C:65:LEU:HD23	1:C:65:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ILE:HG21	1:C:429:PHE:HA	2.02	0.41
1:E:192:SER:HA	1:E:220:LYS:HD3	2.01	0.41
1:E:269:ARG:HA	1:E:389:LYS:HZ3	1.84	0.41
1:D:65:LEU:HD23	1:D:65:LEU:C	2.46	0.41
1:B:378:THR:HB	1:B:383:SER:OG	2.21	0.41
1:C:191:ALA:C	1:C:194:ILE:HD11	2.46	0.41
1:C:372:PRO:HD2	1:C:448:VAL:O	2.20	0.41
1:D:57:THR:HG22	1:D:59:LYS:HG3	2.03	0.41
1:D:311:LEU:HD21	1:D:328:MET:HE2	2.02	0.41
1:G:227:LEU:CD2	1:G:247:LEU:HD21	2.47	0.41
1:C:54:MET:HE3	1:C:61:ALA:H	1.85	0.41
1:G:48:GLN:HG2	3:G:617:HOH:O	2.21	0.40
1:A:143:ILE:HD12	1:A:143:ILE:N	2.36	0.40
1:B:307:ASP:HA	1:B:413:LYS:HB2	2.02	0.40
1:H:92:THR:C	1:H:105:MET:HG3	2.46	0.40
1:C:191:ALA:O	1:C:194:ILE:HD13	2.21	0.40
1:B:66:ASP:OD1	1:B:220:LYS:NZ	2.55	0.40
1:H:1:MET:HG3	1:H:2:LYS:H	1.87	0.40
1:C:74:THR:O	1:C:155:ASN:HA	2.21	0.40
1:D:431:ARG:HH21	1:D:435:GLU:CD	2.29	0.40
1:B:14:THR:HB	1:B:23:MET:CE	2.51	0.40
1:F:74:THR:O	1:F:155:ASN:HA	2.21	0.40
1:G:65:LEU:HD23	1:G:65:LEU:C	2.46	0.40
1:H:94:THR:O	1:H:107:ALA:HA	2.22	0.40
1:H:355:THR:HA	1:H:462:THR:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:GLU:OE2	1:C:79:GLY:H[2_554]	1.56	0.04

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	458/470 (97%)	449 (98%)	9 (2%)	0	100	100
1	B	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	C	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	D	458/470 (97%)	449 (98%)	9 (2%)	0	100	100
1	E	458/470 (97%)	451 (98%)	7 (2%)	0	100	100
1	F	457/470 (97%)	444 (97%)	11 (2%)	2 (0%)	30	28
1	G	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	H	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
All	All	3663/3760 (97%)	3593 (98%)	68 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	459	SER
1	F	422	GLU

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	379/390 (97%)	373 (98%)	6 (2%)	55	64
1	B	382/390 (98%)	377 (99%)	5 (1%)	61	69
1	C	379/390 (97%)	374 (99%)	5 (1%)	61	69
1	D	381/390 (98%)	377 (99%)	4 (1%)	68	76
1	E	382/390 (98%)	377 (99%)	5 (1%)	61	69
1	F	379/390 (97%)	374 (99%)	5 (1%)	61	69
1	G	382/390 (98%)	380 (100%)	2 (0%)	81	88
1	H	381/390 (98%)	375 (98%)	6 (2%)	55	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3045/3120 (98%)	3007 (99%)	38 (1%)	63	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	129	LEU
1	A	208	LYS
1	A	289	ARG
1	A	319	LYS
1	A	421	LYS
1	E	13	LYS
1	E	18	GLU
1	E	214	ASN
1	E	289	ARG
1	E	421	LYS
1	D	104	GLU
1	D	129	LEU
1	D	421	LYS
1	D	431	ARG
1	G	289	ARG
1	G	422	GLU
1	B	23	MET
1	B	257	ILE
1	B	360	ARG
1	B	422	GLU
1	B	461	THR
1	F	119	VAL
1	F	360	ARG
1	F	431	ARG
1	F	439	GLN
1	F	459	SER
1	H	13	LYS
1	H	111	GLU
1	H	119	VAL
1	H	286	LYS
1	H	421	LYS
1	H	459	SER
1	C	119	VAL
1	C	262	MET
1	C	418	GLN
1	C	421	LYS

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Mol	Chain	Res	Type
1	C	461	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	37	HIS
1	E	45	GLN
1	E	81	ASN
1	E	184	GLN
1	E	216	HIS
1	E	418	GLN
1	D	37	HIS
1	G	45	GLN
1	G	155	ASN
1	G	214	ASN
1	G	439	GLN
1	B	37	HIS
1	B	45	GLN
1	B	407	HIS
1	B	418	GLN
1	F	48	GLN
1	F	210	HIS
1	F	287	ASN
1	F	418	GLN
1	H	45	GLN
1	H	210	HIS
1	H	224	GLN
1	H	379	GLN
1	C	37	HIS
1	C	45	GLN
1	C	81	ASN
1	C	159	ASN
1	C	210	HIS
1	C	224	GLN
1	C	407	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
2	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	G	501	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	H	501	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	C	501	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	E	501	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.17	0
2	SO4	F	501	-	4,4,4	0.20	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	SO4	1	0
2	H	501	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	1	0
2	A	501	SO4	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	462/470 (98%)	0.76	71 (15%) 5 5	15, 31, 62, 77	0
1	B	462/470 (98%)	0.25	9 (1%) 66 69	14, 25, 39, 54	0
1	C	462/470 (98%)	0.52	23 (4%) 34 36	16, 31, 48, 58	0
1	D	462/470 (98%)	0.36	16 (3%) 47 49	14, 27, 42, 62	0
1	E	462/470 (98%)	0.30	12 (2%) 57 60	13, 25, 41, 58	0
1	F	461/470 (98%)	0.86	76 (16%) 4 4	15, 31, 67, 80	0
1	G	462/470 (98%)	0.33	15 (3%) 50 53	14, 27, 43, 57	0
1	H	462/470 (98%)	0.51	21 (4%) 38 40	13, 31, 46, 74	0
All	All	3695/3760 (98%)	0.49	243 (6%) 24 26	13, 28, 51, 80	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ILE	6.9
1	A	112	GLY	5.9
1	A	136	ALA	5.7
1	F	83	VAL	5.1
1	F	193	PHE	4.9
1	A	105	MET	4.8
1	F	100	ILE	4.8
1	F	134	VAL	4.7
1	C	1	MET	4.5
1	F	77	LEU	4.5
1	F	106	VAL	4.5
1	F	136	ALA	4.5
1	F	85	LEU	4.4
1	G	104	GLU	4.4
1	H	344	GLU	4.2
1	F	91	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	80	GLY	4.2
1	F	166	ALA	4.2
1	G	456	LEU	4.1
1	F	94	THR	4.1
1	F	92	THR	4.1
1	F	88	GLY	4.0
1	F	139	GLY	4.0
1	F	99	VAL	4.0
1	F	108	VAL	4.0
1	F	143	ILE	4.0
1	G	356	GLU	3.9
1	A	83	VAL	3.8
1	F	146	VAL	3.8
1	A	143	ILE	3.8
1	A	94	THR	3.8
1	F	286	LYS	3.8
1	F	137	ILE	3.7
1	H	172	GLU	3.7
1	D	459	SER	3.7
1	F	422	GLU	3.7
1	A	170	LEU	3.6
1	A	178	LEU	3.6
1	A	113	PHE	3.6
1	A	99	VAL	3.5
1	A	74	THR	3.5
1	H	100	ILE	3.4
1	D	59	LYS	3.4
1	F	37	HIS	3.4
1	G	100	ILE	3.4
1	E	271	ARG	3.4
1	E	337	ARG	3.4
1	A	173	LYS	3.4
1	F	93	PHE	3.4
1	H	114	THR	3.3
1	A	106	VAL	3.3
1	A	142	VAL	3.3
1	F	104	GLU	3.3
1	A	98	SER	3.3
1	F	169	ALA	3.3
1	F	86	LYS	3.3
1	G	60	THR	3.3
1	F	84	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	95	THR	3.2
1	B	46	ARG	3.2
1	F	105	MET	3.2
1	D	342	ARG	3.2
1	A	77	LEU	3.2
1	A	153	GLY	3.2
1	D	356	GLU	3.2
1	C	139	GLY	3.2
1	F	147	LEU	3.1
1	F	150	GLY	3.1
1	A	137	ILE	3.1
1	A	79	GLY	3.1
1	F	424	THR	3.1
1	F	423	ILE	3.1
1	F	81	ASN	3.1
1	F	76	LYS	3.1
1	G	1	MET	3.0
1	A	131	GLY	3.0
1	F	171	ALA	3.0
1	A	84	SER	3.0
1	A	147	LEU	3.0
1	C	343	LEU	3.0
1	A	320	TYR	3.0
1	A	75	MET	3.0
1	G	379	GLN	3.0
1	F	70	PRO	2.9
1	A	140	ASN	2.9
1	A	101	GLY	2.9
1	D	249	VAL	2.9
1	F	133	GLU	2.9
1	F	344	GLU	2.9
1	C	86	LYS	2.9
1	F	142	VAL	2.9
1	A	114	THR	2.9
1	H	105	MET	2.9
1	C	167	LEU	2.8
1	G	99	VAL	2.8
1	F	120	GLY	2.8
1	A	146	VAL	2.8
1	A	421	LYS	2.8
1	A	15	GLU	2.8
1	A	92	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	458	PRO	2.8
1	E	424	THR	2.8
1	F	103	SER	2.7
1	A	85	LEU	2.7
1	E	458	PRO	2.7
1	F	379	GLN	2.7
1	G	460	GLY	2.7
1	F	115	THR	2.7
1	E	52	ASN	2.7
1	E	344	GLU	2.7
1	A	317	LYS	2.7
1	H	319	LYS	2.7
1	A	97	LYS	2.6
1	F	119	VAL	2.6
1	F	80	GLY	2.6
1	F	421	LYS	2.6
1	C	84	SER	2.6
1	H	337	ARG	2.6
1	C	134	VAL	2.6
1	F	144	CYS	2.6
1	A	1	MET	2.6
1	B	344	GLU	2.5
1	A	108	VAL	2.5
1	F	320	TYR	2.5
1	A	109	THR	2.5
1	F	82	ASP	2.5
1	F	107	ALA	2.5
1	A	91	PHE	2.5
1	F	113	PHE	2.5
1	A	423	ILE	2.5
1	A	110	TYR	2.5
1	F	456	LEU	2.5
1	E	289	ARG	2.5
1	C	193	PHE	2.5
1	A	248	GLY	2.5
1	A	155	ASN	2.5
1	C	119	VAL	2.4
1	A	116	ASP	2.4
1	D	101	GLY	2.4
1	D	344	GLU	2.4
1	H	72	ILE	2.4
1	A	87	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	117	LEU	2.4
1	A	93	PHE	2.4
1	A	13	LYS	2.4
1	A	107	ALA	2.4
1	F	152	LEU	2.4
1	A	246	ASP	2.4
1	D	271	ARG	2.4
1	H	1	MET	2.4
1	F	311	LEU	2.3
1	F	153	GLY	2.3
1	A	353	ARG	2.3
1	H	459	SER	2.3
1	A	95	THR	2.3
1	F	90	THR	2.3
1	C	90	THR	2.3
1	A	138	GLU	2.3
1	A	171	ALA	2.3
1	C	169	ALA	2.3
1	E	343	LEU	2.3
1	D	456	LEU	2.3
1	C	85	LEU	2.3
1	D	404	LYS	2.3
1	F	141	LYS	2.3
1	C	208	LYS	2.3
1	A	164	SER	2.3
1	D	423	ILE	2.3
1	A	135	THR	2.3
1	F	135	THR	2.3
1	F	337	ARG	2.3
1	B	286	LYS	2.3
1	H	262	MET	2.3
1	A	78	GLU	2.3
1	F	111	GLU	2.3
1	A	134	VAL	2.3
1	C	449	VAL	2.3
1	A	122	THR	2.3
1	G	462	THR	2.3
1	C	94	THR	2.3
1	H	171	ALA	2.3
1	B	38	GLY	2.3
1	H	110	TYR	2.3
1	H	98	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	317	LYS	2.2
1	F	313	GLY	2.2
1	F	318	GLY	2.2
1	H	316	ALA	2.2
1	E	432	LEU	2.2
1	C	170	LEU	2.2
1	B	104	GLU	2.2
1	A	81	ASN	2.2
1	A	165	ILE	2.2
1	G	358	VAL	2.2
1	A	111	GLU	2.2
1	A	316	ALA	2.2
1	F	73	ARG	2.2
1	H	458	PRO	2.2
1	B	446	GLY	2.2
1	C	353	ARG	2.2
1	A	96	ASP	2.2
1	A	257	ILE	2.1
1	A	344	GLU	2.1
1	D	79	GLY	2.1
1	G	380	GLY	2.1
1	C	152	LEU	2.1
1	F	1	MET	2.1
1	D	139	GLY	2.1
1	F	41	ALA	2.1
1	H	87	ALA	2.1
1	B	262	MET	2.1
1	F	75	MET	2.1
1	F	121	ASN	2.1
1	F	140	ASN	2.1
1	F	110	TYR	2.1
1	G	48	GLN	2.1
1	G	423	ILE	2.1
1	H	128	GLY	2.1
1	C	162	GLY	2.1
1	G	429	PHE	2.1
1	B	358	VAL	2.1
1	F	117	LEU	2.1
1	F	170	LEU	2.1
1	F	432	LEU	2.1
1	C	227	LEU	2.1
1	F	71	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	79	GLY	2.1
1	D	100	ILE	2.1
1	D	53	VAL	2.1
1	H	134	VAL	2.1
1	F	151	ASP	2.0
1	E	431	ARG	2.0
1	A	12	PRO	2.0
1	A	318	GLY	2.0
1	B	80	GLY	2.0
1	A	125	VAL	2.0
1	F	235	GLU	2.0
1	H	138	GLU	2.0
1	E	1	MET	2.0
1	E	459	SER	2.0
1	C	282	ASP	2.0
1	H	13	LYS	2.0
1	A	115	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	501	5/5	0.96	0.10	23,24,31,31	0
2	SO4	D	501	5/5	0.96	0.10	27,29,30,31	0
2	SO4	E	501	5/5	0.97	0.07	21,23,26,27	0
2	SO4	F	501	5/5	0.97	0.06	20,22,24,25	0
2	SO4	H	501	5/5	0.97	0.06	24,27,33,33	0
2	SO4	G	501	5/5	0.98	0.06	22,23,24,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	501	5/5	0.98	0.06	24,26,27,30	0
2	SO4	C	501	5/5	0.98	0.06	22,25,27,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.