



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:45 pm GMT

PDB ID : 3L76
Title : Crystal Structure of Aspartate Kinase from Synechocystis
Authors : Robin, A.; Cobessi, D.; Curien, G.; Robert-Genthon, M.; Ferrer, J.-L.; Dumas, R.
Deposited on : 2009-12-28
Resolution : 2.54 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.

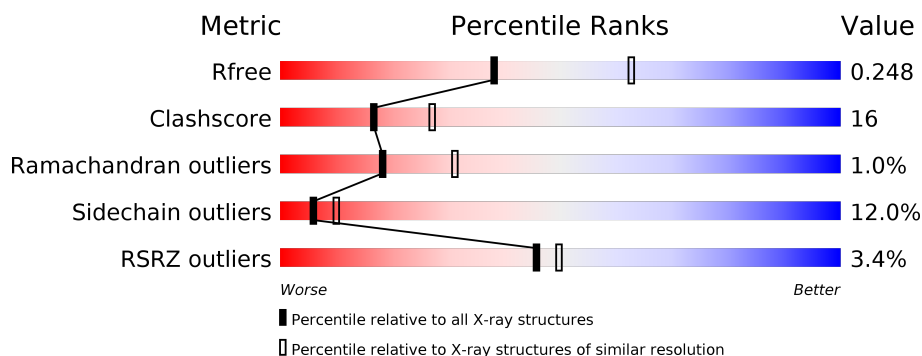
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

i

X-RAY DIFFRACTION

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}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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	600	<div> <div></div> <div>68%</div> <div>25%</div> <div>• •</div> </div>
1	B	600	<div> <div>5%</div> <div>65%</div> <div>26%</div> <div>6%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	THR	B	601	-	-	X	-

2 Entry composition [i](#)

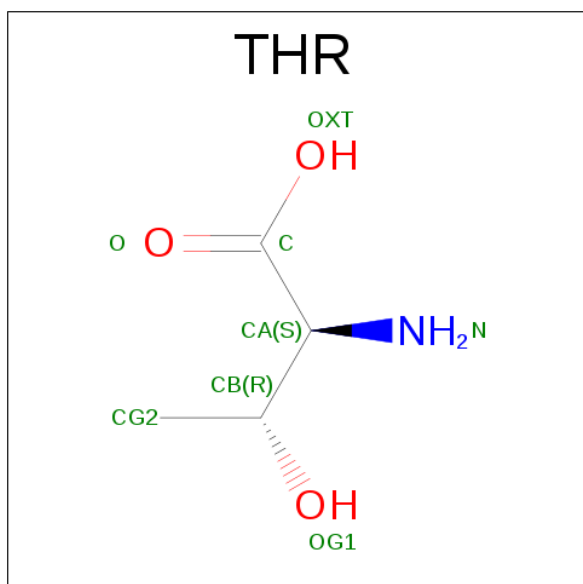
There are 5 unique types of molecules in this entry. The entry contains 8863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aspartokinase.

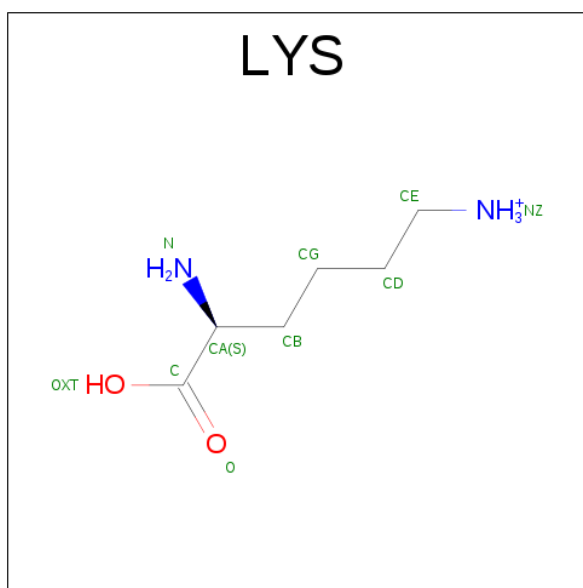
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	12	0
			4335	2723	759	833	20			
1	B	581	Total	C	N	O	S	0	12	0
			4277	2694	735	828	20			

- Molecule 2 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$).



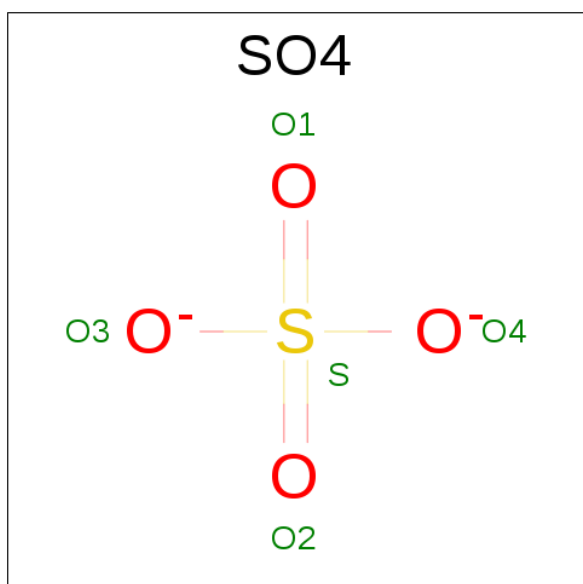
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

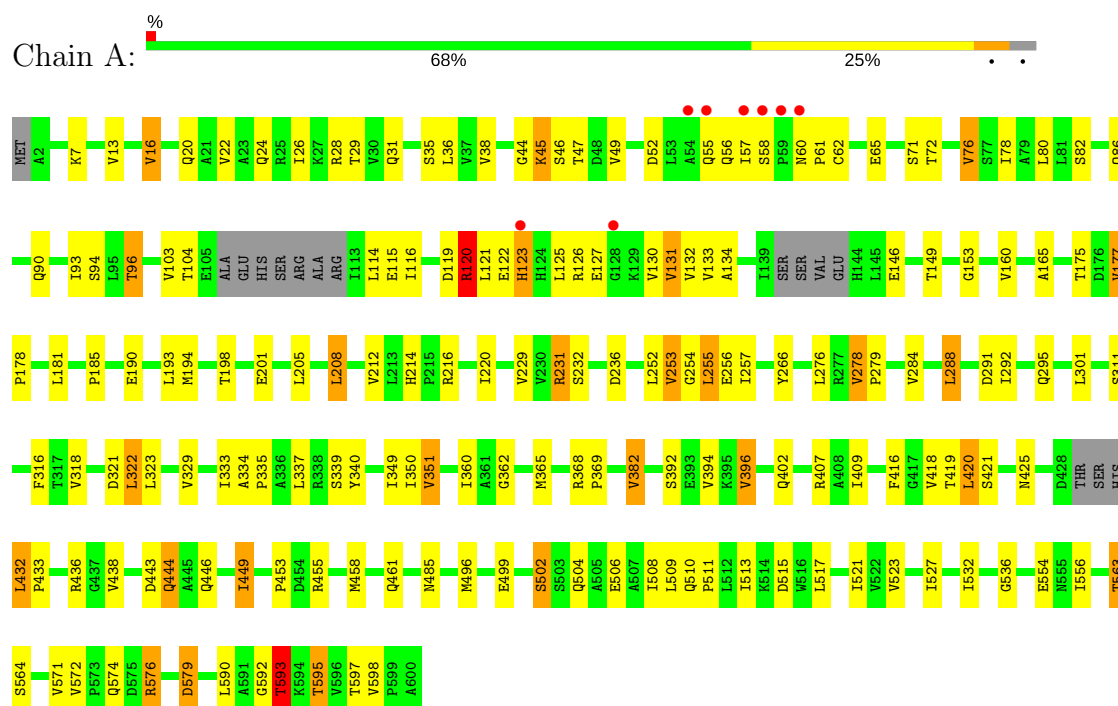
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	101	Total	O	0	0
			101	101		
5	B	73	Total	O	0	0
			73	73		

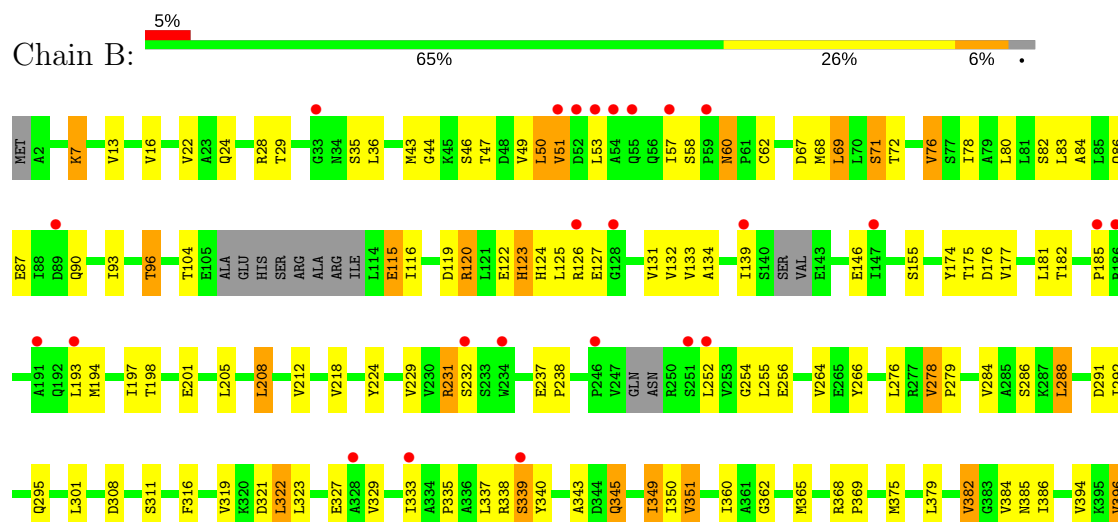
3 Residue-property plots [i](#)

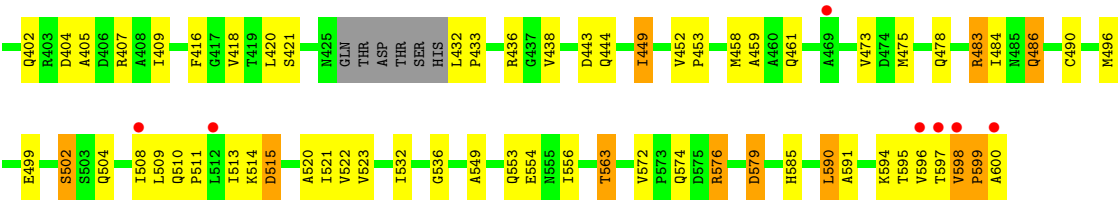
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: Aspartokinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.21Å 237.71Å 150.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.40 – 2.54 41.43 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.40-2.54) 99.7 (41.43-2.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.199 , 0.255 0.190 , 0.248	Depositor DCC
R_{free} test set	2552 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8863	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/4423	0.59	0/6018
1	B	0.40	1/4362 (0.0%)	0.60	0/5939
All	All	0.40	1/8785 (0.0%)	0.59	0/11957

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	CYS	CB-SG	-5.27	1.73	1.81

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	4335	0	4419	133	0
1	B	4277	0	4356	156	0
2	A	16	0	12	0	0
2	B	16	0	12	4	0
3	A	20	0	24	1	0
3	B	20	0	24	1	0
4	A	5	0	0	0	0
5	A	101	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	73	0	0	6	0
All	All	8863	0	8847	277	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 16.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HH21	1:B:131:VAL:HG23	1.19	1.03
1:B:264[B]:VAL:HG13	1:B:420:LEU:HD23	1.54	0.89
1:A:126:ARG:HH21	1:A:131:VAL:HG13	1.42	0.85
1:A:58:SER:HB2	1:B:87:GLU:HG2	1.60	0.84
1:A:201:GLU:OE2	1:A:436:ARG:HD2	1.81	0.80
1:A:323:LEU:HD11	1:A:351:VAL:CG2	2.12	0.80
1:A:80:LEU:HD12	1:B:57:ILE:HD12	1.66	0.77
1:A:126:ARG:HH21	1:A:131:VAL:CG1	1.98	0.76
1:A:252:LEU:HD11	1:A:255:LEU:HG	1.67	0.76
1:A:52:ASP:O	1:A:56:GLN:HG3	1.85	0.76
1:B:76:VAL:HG23	1:B:80:LEU:HD23	1.68	0.73
1:A:35:SER:HB3	1:A:126:ARG:HH11	1.54	0.73
1:B:478:GLN:OE1	2:B:601:THR:HG21	1.89	0.72
1:B:590:LEU:HB3	5:B:667:HOH:O	1.89	0.71
1:A:45:LYS:O	1:A:49:VAL:HG23	1.91	0.71
1:A:120:ARG:HB2	1:A:123:HIS:HB2	1.71	0.71
1:B:323:LEU:HD11	1:B:351:VAL:HG22	1.72	0.71
1:B:224:TYR:HE1	1:B:252:LEU:HB2	1.56	0.70
1:A:323:LEU:HD11	1:A:351:VAL:HG22	1.72	0.70
1:B:264[B]:VAL:HG13	1:B:420:LEU:CD2	2.20	0.70
1:B:50:LEU:HG	1:B:69:LEU:HD22	1.73	0.69
1:A:432:LEU:HD13	1:A:433:PRO:HD2	1.74	0.69
1:B:590:LEU:HD13	1:B:591:ALA:N	2.07	0.68
1:B:386:ILE:HB	2:B:601:THR:HG22	1.75	0.68
1:A:35:SER:HB3	1:A:126:ARG:NH1	2.09	0.67
1:A:120:ARG:O	1:A:120:ARG:HG2	1.94	0.67
1:B:276:LEU:HD11	1:B:350:ILE:HD13	1.77	0.66
1:B:556:ILE:HG12	1:B:576[A]:ARG:HG2	1.77	0.66
1:A:119[A]:ASP:HB3	1:A:120:ARG:HE	1.61	0.66
1:A:253:VAL:HG12	1:A:254:GLY:N	2.10	0.65
1:A:556:ILE:HG12	1:A:576:ARG:HG2	1.77	0.65
1:A:76:VAL:HG12	1:B:72:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576[B]:ARG:NH1	1:B:576[B]:ARG:HB2	2.12	0.65
1:A:266:TYR:CG	1:A:409:ILE:HD11	2.31	0.65
1:A:554:GLU:O	1:A:576:ARG:NH2	2.30	0.64
1:A:57:ILE:O	1:B:87:GLU:HG3	1.96	0.64
1:B:182:THR:HA	1:B:194:MET:HE2	1.77	0.64
1:B:201:GLU:OE2	1:B:436:ARG:HD2	1.98	0.64
1:A:229:VAL:HG11	1:A:231[B]:ARG:HD2	1.80	0.63
1:B:126:ARG:NH2	1:B:131:VAL:HG23	2.04	0.63
1:A:362:GLY:C	1:A:394[A]:VAL:HG23	2.19	0.63
1:A:93:ILE:HD13	1:A:125:LEU:HD13	1.81	0.63
1:B:266:TYR:HB2	1:B:409[A]:ILE:HG21	1.79	0.63
1:B:237[A]:GLU:HG2	1:B:238:PRO:HD2	1.80	0.63
1:B:67:ASP:O	1:B:71:SER:HB3	1.99	0.62
1:B:323:LEU:HD11	1:B:351:VAL:CG2	2.30	0.62
1:B:556:ILE:HG12	1:B:576[B]:ARG:HG2	1.81	0.62
1:A:278:VAL:HG22	1:A:279:PRO:HD2	1.80	0.62
1:A:44:GLY:C	1:A:46:SER:H	2.04	0.61
1:B:60:ASN:O	1:B:60:ASN:ND2	2.30	0.61
1:B:301:LEU:HA	1:B:563:THR:HG21	1.82	0.61
1:A:433:PRO:O	1:A:536:GLY:HA3	2.00	0.61
1:A:392:SER:O	3:A:604:LYS:NZ	2.33	0.61
1:B:340:TYR:CE2	1:B:343:ALA:HB2	2.35	0.61
1:B:93:ILE:HD13	1:B:125:LEU:HD13	1.83	0.61
1:B:205:LEU:HD22	1:B:208:LEU:HD22	1.81	0.60
1:A:278:VAL:O	1:A:311:SER:HB2	2.01	0.60
1:A:119[B]:ASP:HB2	1:A:120:ARG:HE	1.65	0.60
1:B:35:SER:HB3	1:B:126:ARG:HH11	1.67	0.59
1:B:291:ASP:HB2	1:B:333:ILE:CD1	2.32	0.59
1:B:47:THR:O	1:B:51:VAL:HG12	2.01	0.59
1:A:438:VAL:HG12	1:A:532:ILE:HG22	1.84	0.59
1:A:13:VAL:O	1:A:13:VAL:CG1	2.50	0.59
1:A:126:ARG:NH2	1:A:131:VAL:HG13	2.16	0.59
1:B:29:THR:HG22	1:B:36:LEU:HD11	1.85	0.58
1:B:13:VAL:HG12	1:B:13:VAL:O	2.02	0.58
1:A:29:THR:HG22	1:A:36:LEU:HD11	1.86	0.58
1:B:278[A]:VAL:HG22	1:B:279:PRO:HD2	1.85	0.58
1:A:13:VAL:O	1:A:13:VAL:HG12	2.03	0.58
1:B:13:VAL:CG1	1:B:13:VAL:O	2.51	0.58
1:B:486:GLN:HA	1:B:486:GLN:OE1	2.04	0.57
1:B:181:LEU:HD13	1:B:185:PRO:HG3	1.87	0.57
1:B:483[B]:ARG:NH2	5:B:632:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HD13	1:A:134:ALA:HB3	1.85	0.57
1:B:49:VAL:O	1:B:53:LEU:HD13	2.04	0.57
1:B:131:VAL:HG12	1:B:133:VAL:HG23	1.87	0.56
1:B:585:HIS:CB	1:B:590:LEU:HG	2.35	0.56
1:A:382:VAL:O	1:A:407[B]:ARG:NH1	2.39	0.56
1:A:181:LEU:HD13	1:A:185:PRO:HG3	1.88	0.56
1:A:96:THR:HG22	1:B:146:GLU:HG3	1.88	0.56
1:A:510[B]:GLN:HB3	1:A:511:PRO:HD3	1.87	0.55
1:A:94:SER:HB2	1:B:68:MET:HE1	1.89	0.55
1:B:295:GLN:HG3	1:B:329:VAL:HG21	1.89	0.55
1:B:362:GLY:C	1:B:394[A]:VAL:HG23	2.26	0.55
1:A:76:VAL:O	1:A:80:LEU:HD23	2.07	0.55
1:A:229:VAL:HG12	1:A:231[B]:ARG:HG3	1.88	0.54
1:B:197:ILE:HA	1:B:436:ARG:HD3	1.89	0.54
1:B:264[B]:VAL:CG1	1:B:420:LEU:HD23	2.35	0.54
1:A:58:SER:CB	1:B:87:GLU:HG2	2.35	0.54
1:B:116:ILE:CG2	1:B:255:LEU:HB3	2.38	0.54
1:A:205:LEU:HD22	1:A:208:LEU:HD22	1.90	0.53
1:A:301:LEU:HA	1:A:563:THR:HG21	1.89	0.53
1:B:78:ILE:HD13	1:B:134:ALA:HB3	1.90	0.53
1:A:392:SER:HB3	1:A:564:SER:HB3	1.91	0.53
1:A:153:GLY:HA2	1:A:214[A]:HIS:CE1	2.44	0.53
1:A:449:ILE:HD13	1:A:513:ILE:HG21	1.91	0.53
1:A:592:GLY:O	1:A:593:THR:HG23	2.09	0.53
1:B:122:GLU:HB2	1:B:131:VAL:HG21	1.91	0.53
1:B:35:SER:HB3	1:B:126:ARG:NH1	2.24	0.52
1:A:295:GLN:HG3	1:A:329:VAL:HG21	1.90	0.52
1:A:291:ASP:HB2	1:A:333:ILE:CD1	2.40	0.51
1:A:78:ILE:HB	1:A:132:VAL:HG12	1.92	0.51
1:A:229:VAL:CG1	1:A:231[B]:ARG:HD2	2.39	0.51
1:B:237[A]:GLU:CG	1:B:238:PRO:HD2	2.41	0.51
1:B:78:ILE:HB	1:B:132:VAL:HG12	1.91	0.51
1:A:96:THR:HA	1:A:134:ALA:O	2.11	0.51
1:A:504:GLN:O	1:A:508:ILE:HG13	2.11	0.51
1:B:291:ASP:HB2	1:B:333:ILE:HD13	1.93	0.50
1:B:385:ASN:OD1	2:B:601:THR:N	2.44	0.50
1:A:57:ILE:HD12	1:B:80:LEU:HD12	1.92	0.50
1:A:506:GLU:O	1:A:510[A]:GLN:HG3	2.12	0.50
1:B:459:ALA:HB2	2:B:601:THR:HG23	1.93	0.50
1:B:484:ILE:O	1:B:484:ILE:HD12	2.11	0.50
1:A:126:ARG:NH2	1:A:131:VAL:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:GLN:O	1:B:508:ILE:HG13	2.11	0.50
1:B:576[B]:ARG:HH11	1:B:576[B]:ARG:HB2	1.76	0.49
1:A:432:LEU:HD13	1:A:433:PRO:CD	2.41	0.49
1:A:563:THR:HG23	5:A:684:HOH:O	2.13	0.49
1:B:104:THR:HG23	1:B:139:ILE:HG12	1.95	0.49
1:B:174:TYR:CE2	1:B:231:ARG:HD3	2.47	0.49
1:B:438:VAL:HG12	1:B:532:ILE:HG22	1.94	0.49
1:B:345:GLN:H	1:B:345:GLN:CD	2.16	0.49
1:B:327:GLU:HG3	1:B:349:ILE:HD11	1.95	0.49
1:B:46:SER:O	1:B:49:VAL:HG22	2.13	0.49
1:B:510:GLN:HB3	1:B:511:PRO:HD3	1.94	0.49
1:A:276:LEU:HD11	1:A:350:ILE:HD13	1.94	0.49
1:A:44:GLY:C	1:A:46:SER:N	2.66	0.48
1:B:124:HIS:C	1:B:126:ARG:H	2.15	0.48
1:B:126:ARG:NH2	1:B:131:VAL:H	2.11	0.48
1:A:122:GLU:HB2	1:A:131:VAL:HG11	1.96	0.48
1:A:198:THR:OG1	1:A:201:GLU:HG3	2.14	0.48
1:A:288:LEU:HD22	1:A:292:ILE:HD11	1.96	0.48
1:B:104:THR:HG23	1:B:139:ILE:CG1	2.44	0.48
1:B:360:ILE:HD13	1:B:375:MET:HB2	1.95	0.48
1:A:82:SER:O	1:A:86:GLN:HG3	2.14	0.47
1:B:598:VAL:HA	1:B:599:PRO:HD3	1.67	0.47
1:B:176:ASP:O	1:B:177:VAL:HG23	2.14	0.47
1:B:449[A]:ILE:HD12	1:B:520:ALA:O	2.14	0.47
1:B:288:LEU:HD22	1:B:292:ILE:HD11	1.96	0.47
1:A:165:ALA:HB2	1:A:252:LEU:HD23	1.95	0.47
1:A:103:VAL:HG22	1:A:116[A]:ILE:HD13	1.96	0.47
1:A:120:ARG:NE	1:A:120:ARG:N	2.63	0.47
1:A:78:ILE:HG21	1:A:134:ALA:HB2	1.96	0.47
1:B:360:ILE:HG12	1:B:396:VAL:HG13	1.96	0.47
1:B:115:GLU:OE1	1:B:255:LEU:N	2.48	0.47
1:B:368:ARG:HA	1:B:369:PRO:HD3	1.78	0.47
1:B:576[A]:ARG:HG3	1:B:579:ASP:HB2	1.97	0.47
1:A:288:LEU:HD22	1:A:292:ILE:CD1	2.45	0.47
1:B:549:ALA:O	1:B:553:GLN:HG3	2.15	0.47
1:B:76:VAL:HG23	1:B:80:LEU:CD2	2.43	0.47
1:A:120:ARG:HE	1:A:120:ARG:N	2.13	0.47
1:A:301:LEU:O	1:A:316:PHE:HA	2.15	0.47
1:B:453:PRO:O	1:B:458:MET:HG3	2.15	0.47
1:B:96:THR:HA	1:B:134:ALA:O	2.14	0.47
1:A:231[A]:ARG:HH22	1:A:236:ASP:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:O	1:A:502:SER:HB2	2.15	0.46
1:B:288:LEU:HD22	1:B:292:ILE:CD1	2.46	0.46
1:B:231:ARG:HB3	1:B:231:ARG:HH11	1.80	0.46
1:B:590:LEU:C	1:B:590:LEU:HD13	2.35	0.46
1:A:116[B]:ILE:HG22	1:A:257:ILE:CG2	2.45	0.46
1:B:499:GLU:O	1:B:502:SER:HB2	2.16	0.46
1:A:334:ALA:HB3	1:A:335:PRO:HD3	1.98	0.46
1:A:360:ILE:HG12	1:A:396:VAL:HG13	1.98	0.46
1:B:335:PRO:O	1:B:338:ARG:HG3	2.16	0.46
1:A:116[B]:ILE:HG22	1:A:255:LEU:O	2.16	0.46
1:B:181:LEU:HD23	1:B:193:LEU:HA	1.98	0.46
1:A:595:THR:HG22	1:A:595:THR:O	2.16	0.46
1:B:120:ARG:CB	1:B:123:HIS:HB2	2.46	0.45
1:B:514:LYS:HE2	1:B:515:ASP:OD2	2.16	0.45
1:B:78:ILE:HG21	1:B:134:ALA:HB2	1.98	0.45
1:B:301:LEU:HA	1:B:563:THR:CG2	2.46	0.45
1:B:308:ASP:CG	1:B:483[B]:ARG:NH2	2.69	0.45
1:B:181:LEU:CD1	1:B:185:PRO:HG3	2.46	0.45
1:A:279:PRO:O	1:A:284:VAL:HG21	2.16	0.45
1:B:80:LEU:HD13	1:B:80:LEU:HA	1.76	0.45
1:A:574:GLN:C	1:A:576:ARG:H	2.19	0.45
1:B:266:TYR:CE1	1:B:405:ALA:HB1	2.52	0.45
1:B:286:SER:HB2	5:B:609:HOH:O	2.16	0.45
1:A:80:LEU:HD13	1:A:80:LEU:HA	1.77	0.45
1:B:60:ASN:H	1:B:60:ASN:ND2	2.14	0.45
1:A:509:LEU:HB2	1:A:521:ILE:CD1	2.46	0.45
1:A:72:THR:HB	1:B:72:THR:HB	1.99	0.45
1:A:201:GLU:OE2	1:A:436:ARG:CD	2.59	0.45
1:B:433:PRO:O	1:B:536:GLY:HA3	2.17	0.45
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.65	0.44
1:B:432:LEU:HA	1:B:433:PRO:HD3	1.54	0.44
1:B:574:GLN:C	1:B:576[B]:ARG:H	2.19	0.44
1:A:146:GLU:HB2	1:B:96:THR:HG22	1.99	0.44
1:B:554:GLU:O	1:B:576[A]:ARG:NH2	2.46	0.44
1:B:360:ILE:CG1	1:B:396:VAL:HG13	2.47	0.44
1:B:590:LEU:HD12	5:B:674:HOH:O	2.17	0.44
1:A:278:VAL:HG22	1:A:279:PRO:CD	2.46	0.44
1:B:579:ASP:N	1:B:579:ASP:OD1	2.50	0.44
1:B:229:VAL:HG12	1:B:231:ARG:HG3	2.00	0.44
1:B:116:ILE:HG23	1:B:255:LEU:HB3	1.98	0.44
1:B:308:ASP:CG	1:B:483[B]:ARG:HH22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:O	1:B:284:VAL:HG21	2.17	0.44
1:B:375:MET:SD	1:B:396:VAL:HG22	2.58	0.44
1:B:404:ASP:OD1	1:B:407:ARG:NH2	2.51	0.44
1:A:181:LEU:HD23	1:A:193:LEU:HA	2.00	0.44
1:A:453:PRO:O	1:A:458:MET:HG3	2.18	0.44
1:B:13:VAL:O	1:B:43:MET:HE3	2.17	0.44
1:B:319:VAL:HG13	5:B:677:HOH:O	2.17	0.44
1:B:291:ASP:HB2	1:B:333:ILE:HD11	2.00	0.43
1:B:82:SER:O	1:B:86:GLN:HG3	2.18	0.43
1:A:291:ASP:HB2	1:A:333:ILE:HD13	1.99	0.43
1:A:29:THR:CG2	1:A:36:LEU:HD11	2.48	0.43
1:A:26:ILE:HD13	1:A:38:VAL:HG21	2.00	0.43
1:B:124:HIS:O	1:B:126:ARG:N	2.52	0.43
1:B:382:VAL:O	1:B:407:ARG:HD2	2.18	0.43
1:A:416:PHE:O	1:A:418:VAL:HG13	2.18	0.43
1:B:44:GLY:C	1:B:46:SER:H	2.21	0.43
1:A:181:LEU:O	1:A:194:MET:HE3	2.19	0.43
1:B:599:PRO:O	1:B:600:ALA:C	2.57	0.43
1:B:322:LEU:HD12	1:B:322:LEU:HA	1.60	0.43
1:A:116[A]:ILE:HG22	1:A:257:ILE:CG2	2.48	0.43
1:A:190:GLU:CD	1:A:190:GLU:H	2.22	0.43
1:B:175:THR:O	1:B:232:SER:HA	2.19	0.43
1:A:146:GLU:HB2	1:B:96:THR:CG2	2.49	0.43
1:A:444:GLN:HG2	1:A:496:MET:HB3	2.01	0.43
1:A:360:ILE:CG1	1:A:396:VAL:HG13	2.49	0.43
1:B:119:ASP:CG	1:B:120:ARG:H	2.22	0.42
1:B:24:GLN:O	1:B:28:ARG:HG3	2.19	0.42
1:B:379:LEU:HB3	1:B:384:VAL:HG22	2.00	0.42
1:A:181:LEU:CD1	1:A:185:PRO:HG3	2.48	0.42
1:B:509:LEU:HB2	1:B:521:ILE:CD1	2.49	0.42
1:A:362:GLY:O	1:A:394[A]:VAL:HG23	2.18	0.42
1:A:16:VAL:O	1:A:20:GLN:HG3	2.20	0.42
1:A:231[A]:ARG:NH2	1:A:236:ASP:HA	2.34	0.42
1:A:334:ALA:CB	1:A:349[A]:ILE:HD11	2.49	0.42
1:A:510[A]:GLN:HB2	1:A:511:PRO:HD3	2.01	0.42
1:B:513:ILE:HD13	1:B:521:ILE:HG13	2.02	0.42
1:B:319:VAL:HG12	1:B:321:ASP:OD1	2.20	0.42
1:B:511:PRO:O	1:B:514:LYS:HG2	2.19	0.42
1:A:563:THR:CG2	5:A:684:HOH:O	2.65	0.42
1:B:362:GLY:O	1:B:365:MET:HG2	2.20	0.42
3:B:604:LYS:N	5:B:651:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455[A]:ARG:CZ	1:A:458:MET:CE	2.98	0.42
1:B:452:VAL:O	1:B:490:CYS:HB2	2.19	0.42
1:A:496:MET:HE1	1:A:571:VAL:HG21	2.02	0.41
1:A:57:ILE:CG2	1:B:84:ALA:HA	2.50	0.41
1:B:29:THR:CG2	1:B:36:LEU:HD11	2.49	0.41
1:B:338:ARG:O	1:B:339:SER:C	2.58	0.41
1:A:104:THR:O	1:A:114:LEU:HA	2.21	0.41
1:A:177:VAL:HA	1:A:178:PRO:HD3	1.84	0.41
1:B:416:PHE:O	1:B:418:VAL:HG13	2.21	0.41
1:B:124:HIS:C	1:B:126:ARG:N	2.73	0.41
1:B:198:THR:OG1	1:B:201:GLU:HG3	2.20	0.41
1:B:405:ALA:O	1:B:409[A]:ILE:HG12	2.20	0.41
1:A:71:SER:HA	1:A:149:THR:HG23	2.02	0.41
1:A:160:VAL:HG12	1:A:220:ILE:HG22	2.03	0.41
1:A:175:THR:O	1:A:232:SER:HA	2.21	0.41
1:A:60:ASN:N	1:A:61:PRO:HD3	2.36	0.41
1:A:329:VAL:O	1:A:333:ILE:HG13	2.21	0.41
1:B:35:SER:C	1:B:36:LEU:HD12	2.41	0.41
1:B:7:LYS:NZ	1:B:155:SER:HB2	2.35	0.41
1:A:420:LEU:HD22	1:A:421:SER:O	2.21	0.40
1:A:432:LEU:HA	1:A:433:PRO:HD3	1.99	0.40
1:B:301:LEU:O	1:B:316:PHE:HA	2.21	0.40
1:B:590:LEU:CD1	1:B:591:ALA:N	2.81	0.40
1:A:368:ARG:HA	1:A:369:PRO:HD3	1.79	0.40
1:A:579:ASP:N	1:A:579:ASP:OD1	2.53	0.40
1:B:264[B]:VAL:HG22	1:B:409[B]:ILE:CD1	2.51	0.40
1:A:24:GLN:O	1:A:28:ARG:HG3	2.21	0.40
1:A:45:LYS:HE2	1:A:45:LYS:N	2.37	0.40
1:B:475:MET:HB2	1:B:496:MET:HE3	2.03	0.40
1:A:446:GLN:HB2	1:A:527:ILE:HD13	2.03	0.40
1:B:301:LEU:HD23	1:B:563:THR:HG22	2.03	0.40
1:A:65:GLU:HB2	1:B:83:LEU:HD21	2.03	0.40
1:A:362:GLY:O	1:A:365:MET:HG2	2.22	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	589/600 (98%)	553 (94%)	29 (5%)	7 (1%)	15	26
1	B	583/600 (97%)	542 (93%)	35 (6%)	6 (1%)	18	31
All	All	1172/1200 (98%)	1095 (93%)	64 (6%)	13 (1%)	18	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ARG
1	A	253	VAL
1	A	425	ASN
1	A	485	ASN
1	B	120	ARG
1	A	593	THR
1	B	339	SER
1	A	255	LEU
1	A	339	SER
1	B	254	GLY
1	B	483[A]	ARG
1	B	483[B]	ARG
1	B	599	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/479 (96%)	401 (88%)	57 (12%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	452/479 (94%)	398 (88%)	54 (12%)	6 10
All	All	910/958 (95%)	799 (88%)	111 (12%)	6 9

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	VAL
1	A	22	VAL
1	A	31	GLN
1	A	45	LYS
1	A	47	THR
1	A	55	GLN
1	A	62	CYS
1	A	76	VAL
1	A	90	GLN
1	A	96	THR
1	A	115	GLU
1	A	120	ARG
1	A	121	LEU
1	A	123	HIS
1	A	127	GLU
1	A	130	VAL
1	A	131	VAL
1	A	133	VAL
1	A	177	VAL
1	A	208	LEU
1	A	212	VAL
1	A	216	ARG
1	A	231[A]	ARG
1	A	231[B]	ARG
1	A	256	GLU
1	A	278	VAL
1	A	288	LEU
1	A	318	VAL
1	A	322	LEU
1	A	337	LEU
1	A	340	TYR
1	A	351	VAL
1	A	382	VAL
1	A	396	VAL
1	A	402[A]	GLN

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Mol	Chain	Res	Type
1	A	402[B]	GLN
1	A	419	THR
1	A	420	LEU
1	A	432	LEU
1	A	443	ASP
1	A	444	GLN
1	A	449	ILE
1	A	461	GLN
1	A	502	SER
1	A	515	ASP
1	A	517	LEU
1	A	523	VAL
1	A	563	THR
1	A	572	VAL
1	A	576	ARG
1	A	579	ASP
1	A	590	LEU
1	A	593	THR
1	A	595	THR
1	A	597	THR
1	A	598	VAL
1	B	7	LYS
1	B	16	VAL
1	B	22	VAL
1	B	50	LEU
1	B	51	VAL
1	B	58	SER
1	B	60	ASN
1	B	69	LEU
1	B	71	SER
1	B	76	VAL
1	B	90	GLN
1	B	96	THR
1	B	115	GLU
1	B	123	HIS
1	B	127	GLU
1	B	208	LEU
1	B	212	VAL
1	B	218	VAL
1	B	231	ARG
1	B	256	GLU
1	B	278[A]	VAL

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Mol	Chain	Res	Type
1	B	278[B]	VAL
1	B	288	LEU
1	B	322	LEU
1	B	337	LEU
1	B	345	GLN
1	B	349	ILE
1	B	351	VAL
1	B	382	VAL
1	B	396	VAL
1	B	402	GLN
1	B	421	SER
1	B	443	ASP
1	B	444	GLN
1	B	449[A]	ILE
1	B	449[B]	ILE
1	B	461	GLN
1	B	473	VAL
1	B	486	GLN
1	B	502	SER
1	B	515	ASP
1	B	522	VAL
1	B	523	VAL
1	B	563	THR
1	B	572	VAL
1	B	576[A]	ARG
1	B	576[B]	ARG
1	B	579	ASP
1	B	590	LEU
1	B	594	LYS
1	B	595	THR
1	B	596	VAL
1	B	597	THR
1	B	598	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	ASN
1	A	557	ASN
1	B	385	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	THR	A	601	-	4,7,7	0.31	0	3,9,9	0.63	0
2	THR	A	602	-	4,7,7	0.58	0	3,9,9	0.36	0
3	LYS	A	603	-	4,9,9	0.55	0	3,10,10	0.47	0
3	LYS	A	604	-	4,9,9	0.28	0	3,10,10	0.26	0
4	SO4	A	605	-	4,4,4	0.31	0	6,6,6	1.14	1 (16%)
2	THR	B	601	-	4,7,7	0.64	0	3,9,9	0.17	0
2	THR	B	602	-	4,7,7	0.74	0	3,9,9	0.60	0
3	LYS	B	603	-	4,9,9	0.37	0	3,10,10	0.59	0
3	LYS	B	604	-	4,9,9	0.30	0	3,10,10	0.40	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
2	THR	A	601	-	-	0/4/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	THR	A	602	-	-	0/4/8/8	0/0/0/0
3	LYS	A	603	-	-	0/5/9/9	0/0/0/0
3	LYS	A	604	-	-	0/5/9/9	0/0/0/0
4	SO4	A	605	-	-	0/0/0/0	0/0/0/0
2	THR	B	601	-	-	0/4/8/8	0/0/0/0
2	THR	B	602	-	-	0/4/8/8	0/0/0/0
3	LYS	B	603	-	-	0/5/9/9	0/0/0/0
3	LYS	B	604	-	-	0/5/9/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	SO4	O4-S-O3	2.04	118.15	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	LYS	1	0
2	B	601	THR	4	0
3	B	604	LYS	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	585/600 (97%)	0.04	8 (1%) 75 77	24, 57, 95, 147	0
1	B	581/600 (96%)	0.12	32 (5%) 26 28	26, 64, 100, 162	0
All	All	1166/1200 (97%)	0.08	40 (3%) 46 50	24, 61, 98, 162	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	ALA	5.0
1	B	55	GLN	4.6
1	B	234	TRP	4.3
1	B	185	PRO	4.1
1	B	251	SER	3.7
1	A	57	ILE	3.4
1	A	55	GLN	3.2
1	B	51	VAL	3.2
1	B	33	GLY	3.0
1	B	596	VAL	3.0
1	B	328	ALA	3.0
1	B	53	LEU	2.9
1	B	128	GLY	2.8
1	B	191	ALA	2.8
1	B	54	ALA	2.8
1	B	597	THR	2.5
1	B	246	PRO	2.5
1	B	252	LEU	2.5
1	A	58	SER	2.5
1	B	193	LEU	2.5
1	B	186	ARG	2.5
1	B	598	VAL	2.4
1	B	508	ILE	2.4
1	B	339	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	89	ASP	2.3
1	B	139	ILE	2.3
1	A	54	ALA	2.3
1	A	59	PRO	2.3
1	B	147	ILE	2.3
1	A	123	HIS	2.2
1	A	60	ASN	2.2
1	B	232	SER	2.2
1	A	128	GLY	2.2
1	B	57	ILE	2.2
1	B	126	ARG	2.1
1	B	512	LEU	2.1
1	B	333	ILE	2.0
1	B	52	ASP	2.0
1	B	469	ALA	2.0
1	B	59	PRO	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
2	THR	A	602	8/8	0.97	0.18	0.78	25,29,34,48	0
3	LYS	A	604	10/10	0.98	0.18	0.31	21,26,42,48	0
2	THR	B	602	8/8	0.95	0.15	0.28	34,42,60,69	0
2	THR	B	601	8/8	0.97	0.14	0.20	22,47,52,56	0
3	LYS	B	603	10/10	0.97	0.14	-0.37	21,36,49,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LYS	B	604	10/10	0.97	0.12	-0.38	28,40,57,65	0
4	SO4	A	605	5/5	0.99	0.13	-0.49	35,39,40,40	5
2	THR	A	601	8/8	0.98	0.12	-1.12	26,37,48,52	0
3	LYS	A	603	10/10	0.96	0.12	-1.16	21,31,39,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.