



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:56 PM GMT

PDB ID : 1EVL
Title : CRYSTAL STRUCTURE OF A TRUNCATED FORM OF THREONYL-
TRNA SYNTHETASE WITH A THREONYL ADENYLATE ANALOG
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Deposited on : 2000-04-20
Resolution : 1.55 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

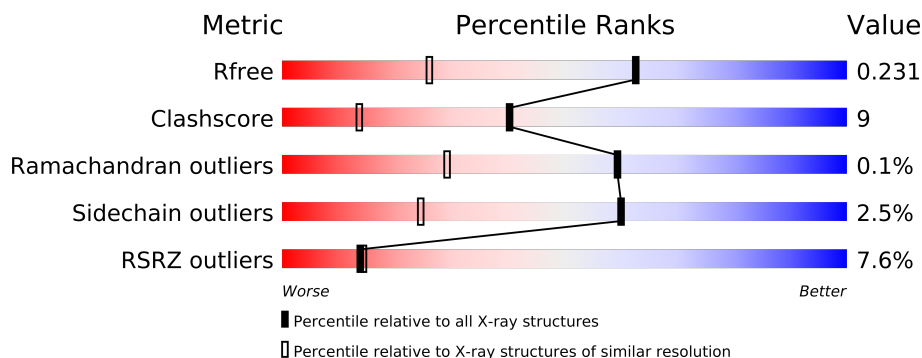
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.55 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}	66092	1117 (1.58-1.54)
Clashscore	79885	1249 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	
1	C	401	
1	D	401	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14730 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

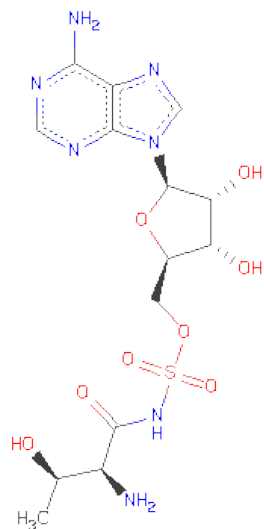
- Molecule 1 is a protein called THREONYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3265	2063	576	603	23			
1	B	401	Total	C	N	O	S	0	0	0
			3268	2064	576	605	23			
1	C	401	Total	C	N	O	S	0	0	0
			3268	2064	576	605	23			
1	D	401	Total	C	N	O	S	0	0	0
			3261	2061	576	601	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (three-letter code: TSB) (formula: C₁₄H₂₁N₇O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	B	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	C	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
3	D	1	Total	C	N	O	S	0	0
			30	14	7	8	1		

- Molecule 4 is water.

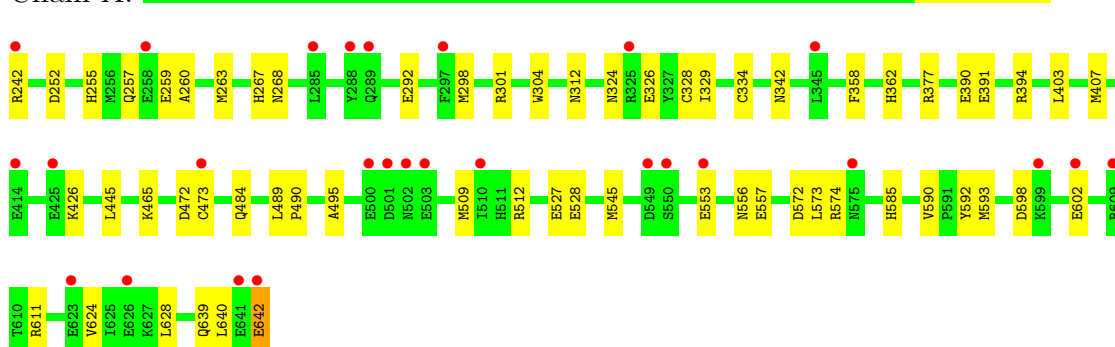
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	395	Total	O	0	0
			395	395		
4	B	390	Total	O	0	0
			390	390		
4	C	397	Total	O	0	0
			397	397		
4	D	362	Total	O	0	0
			362	362		

3 Residue-property plots

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.

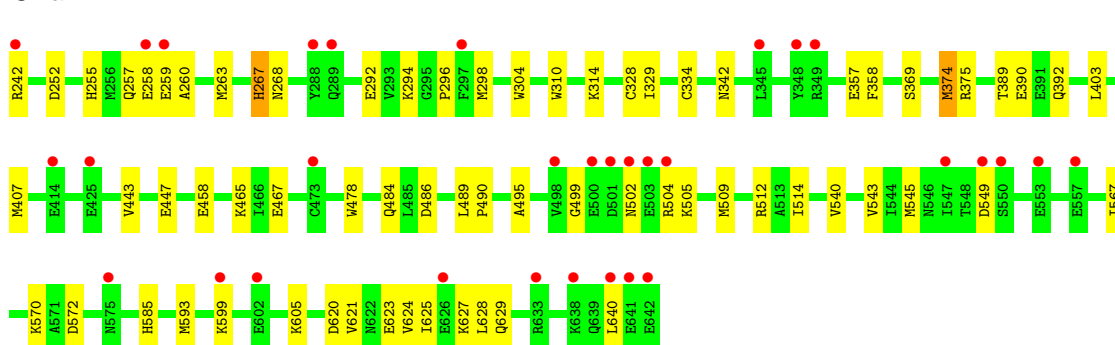
• Molecule 1: THREONYL-TRNA SYNTHETASE

Chain A:



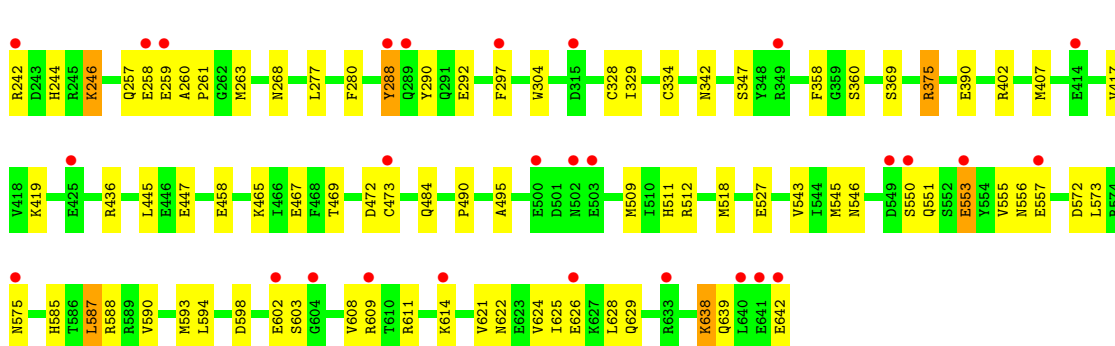
• Molecule 1: THREONYL-TRNA SYNTHETASE

Chain B:



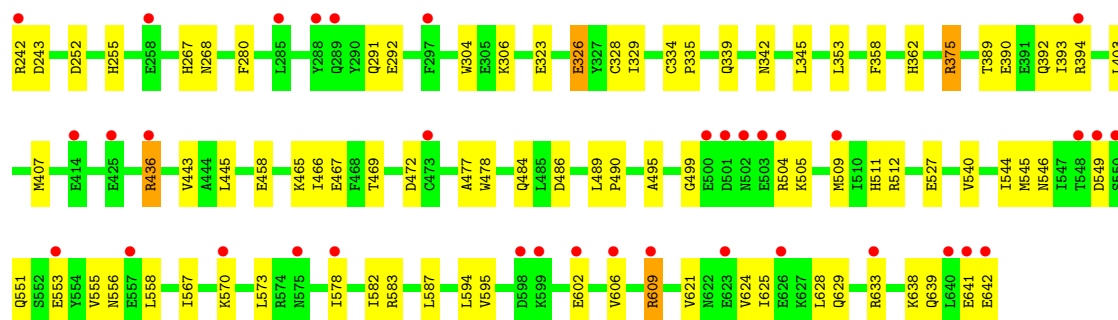
• Molecule 1: THREONYL-TRNA SYNTHETASE

Chain C:



● Molecule 1: THREONYL-TRNA SYNTHETASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 111.10Å 135.20Å 90.00° 93.50° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 29.89 – 1.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.55) 95.5 (29.89-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.54Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.215 , 0.226 0.220 , 0.231	Depositor DCC
R_{free} test set	17612 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 366221 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14730	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 50.85 % 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 6.1009e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/3336	0.63	1/4492 (0.0%)
1	B	0.35	0/3339	0.63	1/4496 (0.0%)
1	C	0.34	0/3339	0.62	1/4496 (0.0%)
1	D	0.35	0/3332	0.63	1/4487 (0.0%)
All	All	0.35	0/13346	0.63	4/17971 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	PHE	N-CA-C	-5.61	95.86	111.00
1	D	358	PHE	N-CA-C	-5.45	96.29	111.00
1	A	358	PHE	N-CA-C	-5.43	96.35	111.00
1	B	358	PHE	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3197	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3268	0	3199	60	0
1	C	3268	0	3199	67	0
1	D	3261	0	3193	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	30	0	21	1	0
3	B	30	0	20	1	0
3	C	30	0	20	1	0
3	D	30	0	21	1	0
4	A	395	0	0	1	0
4	B	390	0	0	4	0
4	C	397	0	0	7	0
4	D	362	0	0	12	0
All	All	14730	0	12870	245	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (245) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:375:ARG:HB2	1:D:375:ARG:HH11	1.03	1.12
1:D:594:LEU:HB3	1:D:606:VAL:HG21	1.36	1.04
1:A:263:MET:HE1	1:B:298:MET:H	1.30	0.93
1:D:582:ILE:HD12	1:D:609:ARG:HD3	1.54	0.90
1:D:375:ARG:CB	1:D:375:ARG:HH11	1.85	0.90
1:D:466:ILE:HG22	4:D:5173:HOH:O	1.72	0.89
1:B:499:GLY:HA3	1:B:505:LYS:HE2	1.55	0.88
1:B:627:LYS:HD3	1:B:640:LEU:HD21	1.53	0.88
1:A:263:MET:CE	1:B:298:MET:H	1.87	0.87
1:D:375:ARG:HB2	1:D:375:ARG:NH1	1.89	0.86
1:A:390:GLU:HG2	1:A:391:GLU:OE2	1.80	0.82
1:D:594:LEU:HB3	1:D:606:VAL:CG2	2.10	0.81
1:B:465:LYS:HB3	1:B:484:GLN:HG2	1.63	0.81
1:A:574:ARG:HG3	1:A:574:ARG:HH11	1.43	0.80
1:B:540:VAL:HG11	1:B:570:LYS:HD3	1.64	0.80
1:B:543:VAL:HG22	1:B:570:LYS:HG3	1.63	0.79
1:A:263:MET:HE2	1:B:298:MET:O	1.84	0.77
1:B:260:ALA:HB1	1:B:263:MET:HB2	1.66	0.75
1:A:263:MET:HE1	1:B:298:MET:N	2.02	0.75
1:A:257:GLN:HE21	1:A:259:GLU:CG	1.99	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:LYS:HG2	1:A:484:GLN:HG2	1.69	0.74
1:A:292:GLU:H	1:B:268:ASN:HD22	1.36	0.74
1:C:614:LYS:HD3	4:C:4209:HOH:O	1.88	0.73
1:C:268:ASN:HD22	1:D:292:GLU:H	1.35	0.72
1:D:393:ILE:HD12	1:D:436:ARG:HH22	1.55	0.72
1:C:246:LYS:HA	1:C:246:LYS:HE3	1.73	0.71
1:C:292:GLU:H	1:D:268:ASN:HD22	1.39	0.71
1:C:484:GLN:HE22	3:C:4002:TSB:HN8	1.38	0.71
1:A:553:GLU:O	1:A:557:GLU:HG3	1.91	0.71
1:A:255:HIS:ND1	1:A:267:HIS:HE1	1.90	0.70
1:D:255:HIS:ND1	1:D:267:HIS:HE1	1.90	0.69
1:B:621:VAL:O	1:B:624:VAL:HG22	1.93	0.69
1:A:329:ILE:HD11	1:B:329:ILE:HD11	1.75	0.68
1:A:268:ASN:HD22	1:B:292:GLU:H	1.41	0.68
1:D:465:LYS:HG2	1:D:484:GLN:HG2	1.76	0.68
1:A:484:GLN:HE22	3:A:2002:TSB:HN8	1.43	0.67
1:D:582:ILE:CD1	1:D:609:ARG:HD3	2.25	0.67
1:B:255:HIS:ND1	1:B:267:HIS:HE1	1.93	0.66
1:C:469:THR:HG22	4:C:4199:HOH:O	1.96	0.66
1:D:390:GLU:H	1:D:390:GLU:CD	1.99	0.65
1:C:553:GLU:O	1:C:557:GLU:HG3	1.97	0.65
1:B:484:GLN:HE22	3:B:3002:TSB:HN8	1.44	0.65
1:B:623:GLU:HG3	1:B:627:LYS:HE2	1.79	0.64
1:B:403:LEU:HG	1:B:407:MET:CE	2.26	0.64
1:B:567:ILE:HD13	1:B:628:LEU:HD12	1.78	0.64
1:C:260:ALA:HB1	1:C:263:MET:HB2	1.79	0.64
1:C:621:VAL:O	1:C:624:VAL:HG22	1.98	0.64
1:B:252:ASP:OD1	1:B:267:HIS:HD2	1.81	0.63
1:D:252:ASP:OD1	1:D:267:HIS:HD2	1.82	0.63
1:C:419:LYS:HE3	1:C:469:THR:HG21	1.81	0.63
1:D:638:LYS:HB2	1:D:642:GLU:HG3	1.81	0.62
1:C:465:LYS:HE3	1:C:467:GLU:OE2	2.00	0.62
1:D:490:PRO:HG3	1:D:509:MET:SD	2.40	0.62
1:A:572:ASP:OD2	1:A:585:HIS:HE1	1.81	0.61
1:A:242:ARG:HD2	1:A:473:CYS:SG	2.41	0.61
1:A:252:ASP:OD1	1:A:267:HIS:HD2	1.83	0.60
1:A:403:LEU:HG	1:A:407:MET:HE3	1.83	0.60
1:D:362:HIS:HD2	4:D:5011:HOH:O	1.85	0.60
1:A:257:GLN:HE21	1:A:259:GLU:HG2	1.67	0.59
1:D:484:GLN:HE22	3:D:5002:TSB:HN8	1.50	0.59
1:A:585:HIS:HD2	4:A:2169:HOH:O	1.86	0.59
1:C:390:GLU:CD	1:C:390:GLU:H	2.04	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:329:ILE:HD11	1:D:329:ILE:HD11	1.83	0.59
1:B:624:VAL:O	1:B:628:LEU:HG	2.03	0.59
1:C:257:GLN:HE21	1:C:259:GLU:CG	2.15	0.58
1:A:390:GLU:H	1:A:390:GLU:CD	2.05	0.58
1:C:638:LYS:HD3	1:C:638:LYS:H	1.69	0.58
1:C:242:ARG:HG3	1:C:473:CYS:HB3	1.86	0.58
1:B:257:GLN:HE21	1:B:259:GLU:HG2	1.69	0.58
1:C:594:LEU:HD22	1:C:608:VAL:HG22	1.85	0.58
1:B:242:ARG:HD2	4:B:3344:HOH:O	2.03	0.57
1:D:558:LEU:HD11	1:D:621:VAL:HG21	1.85	0.57
1:A:598:ASP:O	1:A:602:GLU:HG2	2.04	0.57
1:C:588:ARG:HG3	4:C:4080:HOH:O	2.04	0.57
1:B:572:ASP:OD2	1:B:585:HIS:HE1	1.88	0.57
1:B:627:LYS:CD	1:B:640:LEU:HD21	2.32	0.57
1:C:375:ARG:HH11	1:C:375:ARG:HG2	1.70	0.57
1:D:465:LYS:HD2	1:D:484:GLN:NE2	2.19	0.57
1:B:443:VAL:O	1:B:447:GLU:HG3	2.04	0.56
1:C:572:ASP:OD2	1:C:585:HIS:HE1	1.86	0.56
1:A:324:ASN:ND2	1:D:323:GLU:H	2.02	0.56
1:C:624:VAL:O	1:C:628:LEU:HG	2.05	0.56
1:A:312:ASN:OD1	1:A:426:LYS:HG3	2.06	0.56
1:A:574:ARG:HG3	1:A:574:ARG:NH1	2.19	0.56
1:D:291:GLN:OE1	1:D:353:LEU:HD21	2.06	0.56
1:C:465:LYS:CB	1:C:484:GLN:HG2	2.36	0.56
1:C:417:VAL:HB	1:C:469:THR:OG1	2.05	0.56
1:B:294:LYS:HD2	1:B:357:GLU:OE2	2.05	0.56
1:C:490:PRO:HG3	1:C:509:MET:CE	2.36	0.56
1:C:609:ARG:HD3	1:C:614:LYS:O	2.05	0.56
1:C:280:PHE:CE2	1:C:407:MET:HG2	2.41	0.55
1:D:583:ARG:O	1:D:587:LEU:HD13	2.06	0.55
1:A:624:VAL:O	1:A:628:LEU:HG	2.06	0.55
1:D:345:LEU:HD12	1:D:504:ARG:HH22	1.71	0.55
1:A:592:TYR:OH	1:A:640:LEU:HD13	2.07	0.55
1:B:465:LYS:CB	1:B:484:GLN:HG2	2.35	0.55
1:C:402:ARG:HG3	4:C:4359:HOH:O	2.06	0.55
1:D:465:LYS:CG	1:D:484:GLN:HG2	2.35	0.55
1:D:490:PRO:HG3	1:D:509:MET:HG3	1.88	0.55
1:D:578:ILE:HD11	1:D:595:VAL:HG21	1.88	0.54
1:C:465:LYS:HB3	1:C:484:GLN:HG2	1.88	0.54
1:B:390:GLU:H	1:B:390:GLU:CD	2.09	0.54
1:A:490:PRO:HG3	1:A:509:MET:CE	2.37	0.54
1:B:543:VAL:HG22	1:B:570:LYS:CG	2.35	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:504:ARG:HG2	1:B:504:ARG:HH11	1.72	0.53
1:B:504:ARG:NH1	1:B:504:ARG:HG2	2.23	0.53
1:B:260:ALA:HB1	1:B:263:MET:CB	2.35	0.53
1:D:306:LYS:HE2	4:D:5243:HOH:O	2.08	0.53
1:A:301:ARG:HG3	1:A:328:CYS:SG	2.48	0.53
1:C:268:ASN:ND2	1:D:292:GLU:H	2.05	0.52
1:D:394:ARG:HH21	1:D:443:VAL:HG11	1.75	0.52
1:D:389:THR:OG1	1:D:392:GLN:HG3	2.10	0.52
1:C:277:LEU:HB2	1:C:518:MET:CE	2.40	0.52
1:A:472:ASP:HB2	1:A:527:GLU:OE1	2.08	0.51
1:B:490:PRO:HD3	1:B:509:MET:HE3	1.93	0.51
1:D:545:MET:CE	1:D:595:VAL:HG22	2.40	0.51
1:B:540:VAL:HG11	1:B:570:LYS:CD	2.38	0.51
1:B:304:TRP:CD1	1:B:328:CYS:HB2	2.46	0.51
1:C:556:ASN:HD21	1:C:573:LEU:HD11	1.74	0.51
1:B:374:MET:HG2	1:B:478:TRP:CE2	2.46	0.51
1:D:578:ILE:HD12	1:D:595:VAL:HG11	1.92	0.50
1:D:540:VAL:HG11	1:D:570:LYS:HZ3	1.75	0.50
1:A:298:MET:HG2	1:B:263:MET:CE	2.42	0.50
1:D:469:THR:HG21	1:D:477:ALA:HB1	1.93	0.50
1:A:391:GLU:H	1:A:391:GLU:CD	2.14	0.50
1:B:257:GLN:HE21	1:B:259:GLU:CG	2.25	0.50
1:A:304:TRP:CD1	1:A:328:CYS:HB2	2.47	0.50
1:D:472:ASP:HB2	1:D:527:GLU:OE1	2.11	0.50
1:C:280:PHE:CZ	1:C:407:MET:HG2	2.47	0.50
1:B:342:ASN:HD21	1:B:495:ALA:HA	1.76	0.49
1:D:486:ASP:OD2	1:D:489:LEU:HG	2.13	0.49
1:D:403:LEU:HG	1:D:407:MET:HE3	1.93	0.49
1:D:545:MET:CE	1:D:582:ILE:HD11	2.43	0.49
1:A:292:GLU:H	1:B:268:ASN:ND2	2.07	0.49
1:C:369:SER:O	1:C:375:ARG:HG2	2.13	0.48
1:C:447:GLU:HG2	4:C:4377:HOH:O	2.13	0.48
1:D:602:GLU:HG3	4:D:5308:HOH:O	2.13	0.48
1:C:417:VAL:O	1:C:469:THR:HG23	2.13	0.48
1:C:550:SER:HB3	1:C:551:GLN:NE2	2.28	0.48
1:A:260:ALA:HB1	1:A:263:MET:HB2	1.95	0.48
1:D:553:GLU:HB3	4:D:5077:HOH:O	2.13	0.48
1:D:304:TRP:CD1	1:D:328:CYS:HB2	2.49	0.48
1:A:298:MET:HG2	1:B:263:MET:HE1	1.95	0.47
1:C:258:GLU:O	1:C:261:PRO:HD3	2.14	0.47
1:C:304:TRP:CD1	1:C:328:CYS:HB2	2.49	0.47
1:D:499:GLY:HA3	1:D:505:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:545:MET:HB2	1:D:545:MET:HE3	1.51	0.47
1:D:242:ARG:HA	4:D:5092:HOH:O	2.14	0.47
1:D:545:MET:HE1	1:D:582:ILE:HD11	1.96	0.47
1:B:623:GLU:CG	1:B:627:LYS:HE2	2.43	0.47
1:D:567:ILE:HD13	1:D:628:LEU:HD13	1.97	0.47
1:C:590:VAL:O	1:C:611:ARG:HB3	2.14	0.47
1:D:255:HIS:ND1	1:D:267:HIS:CE1	2.78	0.47
1:D:353:LEU:HD23	4:D:5150:HOH:O	2.14	0.47
1:C:543:VAL:HG11	1:C:585:HIS:CE1	2.50	0.47
1:B:369:SER:O	1:B:375:ARG:HD2	2.15	0.47
1:B:458:GLU:O	1:B:465:LYS:HE2	2.15	0.46
1:D:342:ASN:HD21	1:D:495:ALA:HA	1.80	0.46
1:D:490:PRO:HG3	1:D:509:MET:CG	2.45	0.46
1:A:394:ARG:HB2	1:A:394:ARG:NH1	2.31	0.46
1:A:394:ARG:HB2	1:A:394:ARG:HH11	1.80	0.46
1:B:599:LYS:NZ	1:B:599:LYS:HB2	2.30	0.46
1:C:260:ALA:HB1	1:C:263:MET:CB	2.44	0.46
1:A:545:MET:CE	1:A:593:MET:HB3	2.46	0.46
1:A:263:MET:HE3	1:B:296:PRO:HB2	1.98	0.46
1:B:403:LEU:HG	1:B:407:MET:HE3	1.95	0.46
1:C:545:MET:CE	1:C:593:MET:HB3	2.46	0.46
1:B:407:MET:HE1	1:B:514:ILE:HG13	1.97	0.46
1:C:472:ASP:HB2	1:C:527:GLU:OE1	2.16	0.46
1:C:342:ASN:HD21	1:C:495:ALA:HA	1.79	0.46
1:C:258:GLU:HG3	1:C:259:GLU:OE2	2.16	0.46
1:A:490:PRO:HG3	1:A:509:MET:HE2	1.96	0.46
1:B:625:ILE:O	1:B:629:GLN:HG3	2.16	0.46
1:C:257:GLN:HE21	1:C:259:GLU:HG2	1.78	0.45
1:A:342:ASN:HD21	1:A:495:ALA:HA	1.80	0.45
1:D:375:ARG:NH1	1:D:478:TRP:HZ3	2.15	0.45
1:A:574:ARG:HH11	1:A:574:ARG:CG	2.18	0.45
1:D:544:ILE:HG22	1:D:555:VAL:HG13	1.98	0.45
1:D:639:GLN:O	1:D:642:GLU:HG2	2.17	0.45
1:B:294:LYS:HA	1:B:294:LYS:HD2	1.77	0.45
1:C:490:PRO:HG3	1:C:509:MET:HE2	1.98	0.45
1:A:574:ARG:CG	1:A:574:ARG:NH1	2.78	0.45
1:D:345:LEU:CD1	1:D:504:ARG:NH2	2.80	0.45
1:D:625:ILE:O	1:D:629:GLN:HG3	2.17	0.45
1:C:297:PHE:HE2	1:D:329:ILE:HD13	1.82	0.44
1:C:257:GLN:NE2	1:C:259:GLU:CG	2.80	0.44
1:D:280:PHE:CE2	1:D:407:MET:HG2	2.52	0.44
1:C:625:ILE:O	1:C:629:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:345:LEU:HD12	1:D:504:ARG:NH2	2.33	0.44
1:D:393:ILE:HD12	1:D:436:ARG:NH2	2.27	0.44
1:C:277:LEU:HB2	1:C:518:MET:HE1	1.98	0.44
1:A:268:ASN:ND2	1:B:292:GLU:H	2.13	0.44
1:D:621:VAL:O	1:D:624:VAL:CG1	2.66	0.44
1:B:490:PRO:HG2	4:B:3126:HOH:O	2.17	0.44
1:C:292:GLU:H	1:D:268:ASN:ND2	2.11	0.43
1:C:484:GLN:HB2	1:C:511:HIS:HB2	2.00	0.43
1:B:465:LYS:HE3	1:B:467:GLU:OE2	2.18	0.43
1:C:546:ASN:HB3	1:C:555:VAL:HG21	2.00	0.43
1:B:486:ASP:OD2	1:B:489:LEU:HG	2.18	0.43
1:D:375:ARG:NH1	1:D:478:TRP:CZ3	2.86	0.43
1:C:598:ASP:O	1:C:602:GLU:HG2	2.18	0.43
1:C:622:ASN:O	1:C:626:GLU:HG3	2.18	0.43
1:A:260:ALA:HB1	1:A:263:MET:HG3	2.01	0.43
1:B:389:THR:OG1	1:B:392:GLN:HG3	2.19	0.43
1:D:465:LYS:NZ	4:D:5044:HOH:O	2.47	0.42
1:D:540:VAL:HG11	1:D:570:LYS:NZ	2.34	0.42
1:A:556:ASN:HD21	1:A:573:LEU:HD11	1.84	0.42
1:D:467:GLU:C	4:D:5173:HOH:O	2.58	0.42
1:A:255:HIS:ND1	1:A:267:HIS:CE1	2.79	0.42
1:D:545:MET:HE2	1:D:595:VAL:HG22	2.00	0.42
1:D:436:ARG:HD2	4:D:5191:HOH:O	2.19	0.42
1:A:362:HIS:HA	1:A:377:ARG:O	2.19	0.42
1:C:258:GLU:HG2	4:C:4257:HOH:O	2.20	0.42
1:D:633:ARG:HG2	1:D:633:ARG:NH1	2.35	0.42
1:D:466:ILE:C	4:D:5173:HOH:O	2.58	0.42
1:C:242:ARG:HD3	1:C:527:GLU:O	2.19	0.42
1:A:639:GLN:O	1:A:642:GLU:HG3	2.20	0.42
1:C:244:HIS:HB3	1:C:527:GLU:HG3	2.01	0.42
1:D:621:VAL:O	1:D:624:VAL:HG13	2.20	0.42
1:A:324:ASN:HD21	1:D:323:GLU:H	1.65	0.41
1:A:590:VAL:O	1:A:611:ARG:HB3	2.20	0.41
1:D:469:THR:CG2	1:D:477:ALA:HB1	2.50	0.41
1:C:587:LEU:HA	1:C:587:LEU:HD12	1.83	0.41
1:D:556:ASN:HD21	1:D:573:LEU:HD11	1.85	0.41
1:C:360:SER:N	4:C:4337:HOH:O	2.48	0.41
4:B:3315:HOH:O	1:D:326:GLU:HB2	2.19	0.41
1:B:504:ARG:NH2	4:B:3153:HOH:O	2.53	0.41
1:C:639:GLN:O	1:C:642:GLU:HB2	2.21	0.41
1:B:605:LYS:NZ	1:B:620:ASP:OD1	2.51	0.41
1:A:391:GLU:N	1:A:391:GLU:CD	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:484:GLN:HB2	1:D:511:HIS:HB2	2.02	0.41
1:D:335:PRO:O	1:D:339:GLN:HG2	2.20	0.41
1:A:489:LEU:HB3	1:A:490:PRO:HD3	2.03	0.41
1:C:277:LEU:HB2	1:C:518:MET:HE3	2.02	0.41
1:C:458:GLU:O	1:C:465:LYS:HE2	2.20	0.41
1:D:490:PRO:CG	1:D:509:MET:HG3	2.50	0.41
1:D:578:ILE:O	1:D:582:ILE:HG12	2.21	0.41
1:B:310:TRP:O	1:B:314:LYS:HB2	2.20	0.41
1:C:288:TYR:HB2	1:C:290:TYR:CD1	2.55	0.41
1:B:545:MET:CE	1:B:593:MET:HB3	2.51	0.41
1:A:465:LYS:HE2	1:A:484:GLN:NE2	2.35	0.40
1:C:259:GLU:HB2	4:D:5247:HOH:O	2.21	0.40
1:D:546:ASN:HB2	1:D:551:GLN:HB2	2.01	0.40
1:C:621:VAL:O	1:C:624:VAL:CG2	2.69	0.40
1:D:546:ASN:HB3	1:D:555:VAL:HG21	2.03	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	399/401 (100%)	392 (98%)	7 (2%)	0	100	100
1	B	399/401 (100%)	393 (98%)	6 (2%)	0	100	100
1	C	399/401 (100%)	389 (98%)	9 (2%)	1 (0%)	50	21
1	D	399/401 (100%)	391 (98%)	7 (2%)	1 (0%)	50	21
All	All	1596/1604 (100%)	1565 (98%)	29 (2%)	2 (0%)	59	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	603	SER
1	D	641	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	353/356 (99%)	347 (98%)	6 (2%)	73	42
1	B	354/356 (99%)	347 (98%)	7 (2%)	68	35
1	C	354/356 (99%)	342 (97%)	12 (3%)	49	15
1	D	352/356 (99%)	342 (97%)	10 (3%)	56	20
All	All	1413/1424 (99%)	1378 (98%)	35 (2%)	60	24

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	GLU
1	A	334	CYS
1	A	445	LEU
1	A	512	ARG
1	A	528	GLU
1	A	642	GLU
1	B	258	GLU
1	B	267	HIS
1	B	334	CYS
1	B	374	MET
1	B	502	ASN
1	B	512	ARG
1	B	549	ASP
1	C	246	LYS
1	C	288	TYR
1	C	334	CYS
1	C	347	SER
1	C	375	ARG
1	C	436	ARG
1	C	445	LEU
1	C	512	ARG
1	C	553	GLU
1	C	575	ASN
1	C	587	LEU
1	C	638	LYS
1	D	243	ASP

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Mol	Chain	Res	Type
1	D	326	GLU
1	D	334	CYS
1	D	375	ARG
1	D	436	ARG
1	D	445	LEU
1	D	458	GLU
1	D	512	ARG
1	D	549	ASP
1	D	609	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	257	GLN
1	A	267	HIS
1	A	268	ASN
1	A	289	GLN
1	A	291	GLN
1	A	324	ASN
1	A	342	ASN
1	A	343	GLN
1	A	381	GLN
1	A	455	GLN
1	A	484	GLN
1	A	556	ASN
1	A	585	HIS
1	B	267	HIS
1	B	268	ASN
1	B	291	GLN
1	B	312	ASN
1	B	339	GLN
1	B	342	ASN
1	B	381	GLN
1	B	455	GLN
1	B	502	ASN
1	B	556	ASN
1	B	585	HIS
1	C	268	ASN
1	C	291	GLN
1	C	324	ASN
1	C	342	ASN

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Mol	Chain	Res	Type
1	C	449	ASN
1	C	455	GLN
1	C	556	ASN
1	C	585	HIS
1	D	267	HIS
1	D	268	ASN
1	D	289	GLN
1	D	342	ASN
1	D	362	HIS
1	D	381	GLN
1	D	556	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	TSB	A	2002	2	32,32,32	1.94	4 (12%)	48,48,48	1.00	2 (4%)
3	TSB	B	3002	2	32,32,32	2.05	4 (12%)	48,48,48	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TSB	C	4002	2	32,32,32	2.06	4 (12%)	48,48,48	0.98	3 (6%)
3	TSB	D	5002	2	32,32,32	2.00	4 (12%)	48,48,48	0.99	3 (6%)

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	TSB	A	2002	2	-	0/23/39/39	0/1/3/3
3	TSB	B	3002	2	-	0/23/39/39	0/1/3/3
3	TSB	C	4002	2	-	0/23/39/39	0/1/3/3
3	TSB	D	5002	2	-	0/23/39/39	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5002	TSB	O2S-S1	7.74	1.49	1.42
3	C	4002	TSB	O2S-S1	7.63	1.49	1.42
3	B	3002	TSB	O2S-S1	7.57	1.49	1.42
3	A	2002	TSB	O2S-S1	7.43	1.49	1.42
3	C	4002	TSB	O1S-S1	6.70	1.48	1.42
3	B	3002	TSB	O1S-S1	6.69	1.48	1.42
3	D	5002	TSB	O1S-S1	6.24	1.48	1.42
3	A	2002	TSB	O1S-S1	6.10	1.47	1.42
3	B	3002	TSB	C-N8	-3.84	1.31	1.37
3	C	4002	TSB	C-N8	-3.66	1.31	1.37
3	D	5002	TSB	C-N8	-3.55	1.31	1.37
3	A	2002	TSB	C-N8	-3.33	1.31	1.37
3	C	4002	TSB	CA-C	-2.85	1.49	1.53
3	B	3002	TSB	CA-C	-2.74	1.49	1.53
3	A	2002	TSB	CA-C	-2.36	1.50	1.53
3	D	5002	TSB	CA-C	-2.33	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	TSB	C-N8-S1	-3.13	120.42	124.35
3	A	2002	TSB	C-N8-S1	-2.94	120.66	124.35
3	A	2002	TSB	O2S-S1-O1S	-2.77	118.56	121.45
3	C	4002	TSB	C-N8-S1	-2.73	120.93	124.35
3	D	5002	TSB	O2S-S1-O1S	-2.65	118.69	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	TSB	O2S-S1-O1S	-2.54	118.80	121.45
3	C	4002	TSB	O2S-S1-O1S	-2.50	118.84	121.45
3	D	5002	TSB	C-N8-S1	-2.29	121.48	124.35
3	D	5002	TSB	CB-CA-N	2.17	112.03	109.22
3	B	3002	TSB	CB-CA-N	2.13	111.98	109.22
3	C	4002	TSB	CB-CA-N	2.05	111.89	109.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	401/401 (100%)	0.39	27 (6%) 17 18	11, 19, 30, 36	0
1	B	401/401 (100%)	0.45	32 (7%) 12 13	11, 19, 32, 37	0
1	C	401/401 (100%)	0.45	28 (6%) 16 17	12, 20, 33, 38	0
1	D	401/401 (100%)	0.54	36 (8%) 10 10	12, 20, 33, 37	0
All	All	1604/1604 (100%)	0.46	123 (7%) 14 14	11, 20, 32, 38	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	602	GLU	5.5
1	A	502	ASN	5.2
1	D	640	LEU	5.1
1	D	642	GLU	4.5
1	B	602	GLU	4.5
1	C	642	GLU	4.4
1	A	642	GLU	4.3
1	A	575	ASN	4.3
1	B	502	ASN	4.3
1	D	549	ASP	4.3
1	C	633	ARG	4.2
1	C	549	ASP	4.1
1	C	288	TYR	4.1
1	D	550	SER	4.0
1	A	297	PHE	4.0
1	D	297	PHE	4.0
1	B	640	LEU	3.9
1	C	242	ARG	3.9
1	C	602	GLU	3.9
1	D	599	LYS	3.9
1	D	578	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	242	ARG	3.6
1	B	349	ARG	3.6
1	D	503	GLU	3.5
1	D	575	ASN	3.5
1	A	602	GLU	3.5
1	C	258	GLU	3.5
1	C	502	ASN	3.5
1	D	501	ASP	3.5
1	D	504	ARG	3.4
1	B	503	GLU	3.4
1	D	242	ARG	3.3
1	B	641	GLU	3.3
1	A	641	GLU	3.3
1	C	473	CYS	3.3
1	B	288	TYR	3.3
1	D	641	GLU	3.2
1	C	425	GLU	3.2
1	D	609	ARG	3.2
1	A	473	CYS	3.2
1	A	414	GLU	3.2
1	C	500	GLU	3.2
1	B	642	GLU	3.2
1	A	345	LEU	3.2
1	D	285	LEU	3.1
1	C	349	ARG	3.1
1	D	557	GLU	3.1
1	B	549	ASP	3.1
1	B	258	GLU	3.0
1	D	500	GLU	3.0
1	D	436	ARG	3.0
1	D	633	ARG	3.0
1	A	503	GLU	3.0
1	A	549	ASP	3.0
1	B	500	GLU	3.0
1	A	425	GLU	3.0
1	C	604	GLY	2.9
1	D	425	GLU	2.9
1	C	503	GLU	2.9
1	A	501	ASP	2.9
1	C	575	ASN	2.9
1	B	501	ASP	2.9
1	D	502	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	414	GLU	2.9
1	D	258	GLU	2.9
1	A	258	GLU	2.8
1	D	553	GLU	2.8
1	B	550	SER	2.8
1	A	242	ARG	2.7
1	A	500	GLU	2.7
1	C	640	LEU	2.7
1	D	289	GLN	2.7
1	D	473	CYS	2.7
1	D	288	TYR	2.6
1	C	550	SER	2.6
1	A	289	GLN	2.6
1	C	259	GLU	2.6
1	D	598	ASP	2.6
1	B	547	ILE	2.6
1	C	297	PHE	2.6
1	C	609	ARG	2.5
1	A	288	TYR	2.5
1	A	285	LEU	2.5
1	D	626	GLU	2.5
1	D	509	MET	2.4
1	C	289	GLN	2.4
1	C	553	GLU	2.4
1	B	297	PHE	2.4
1	B	425	GLU	2.4
1	B	626	GLU	2.4
1	C	641	GLU	2.3
1	A	325	ARG	2.3
1	B	473	CYS	2.3
1	B	638	LYS	2.3
1	C	626	GLU	2.3
1	D	548	THR	2.3
1	A	553	GLU	2.2
1	B	498	VAL	2.2
1	A	550	SER	2.2
1	D	414	GLU	2.2
1	B	259	GLU	2.2
1	B	345	LEU	2.2
1	B	575	ASN	2.2
1	B	599	LYS	2.2
1	D	394	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	599	LYS	2.1
1	C	614	LYS	2.1
1	D	606	VAL	2.1
1	B	633	ARG	2.1
1	B	553	GLU	2.1
1	C	557	GLU	2.1
1	D	623	GLU	2.1
1	D	570	LYS	2.1
1	B	504	ARG	2.1
1	B	557	GLU	2.0
1	C	414	GLU	2.0
1	A	609	ARG	2.0
1	C	315	ASP	2.0
1	A	623	GLU	2.0
1	B	289	GLN	2.0
1	A	510	ILE	2.0
1	A	626	GLU	2.0
1	B	348	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	C	1	1/1	0.09	-0.51	13,13,13,13	0
3	TSB	D	5002	30/30	0.11	-0.51	12,14,15,15	0
3	TSB	C	4002	30/30	0.10	-0.52	11,13,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TSB	A	2002	30/30	0.09	-0.61	11,13,14,14	0
2	ZN	D	1	1/1	0.09	-0.94	13,13,13,13	0
3	TSB	B	3002	30/30	0.08	-1.22	10,11,13,14	0
2	ZN	A	1	1/1	0.07	-1.80	12,12,12,12	0
2	ZN	B	1	1/1	0.05	-3.32	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.