



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:46 AM UTC

PDB ID : 4XHA / pdb_00004xha
Title : Crystal structure of Thosea asigna virus RNA-dependent RNA polymerase (RdRP) complexed with Lu3+
Authors : Ferrero, D.S.; Buxaderas, M.; Rodriguez, J.F.; Verdaguer, N.
Deposited on : 2015-01-05
Resolution : 3.00 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

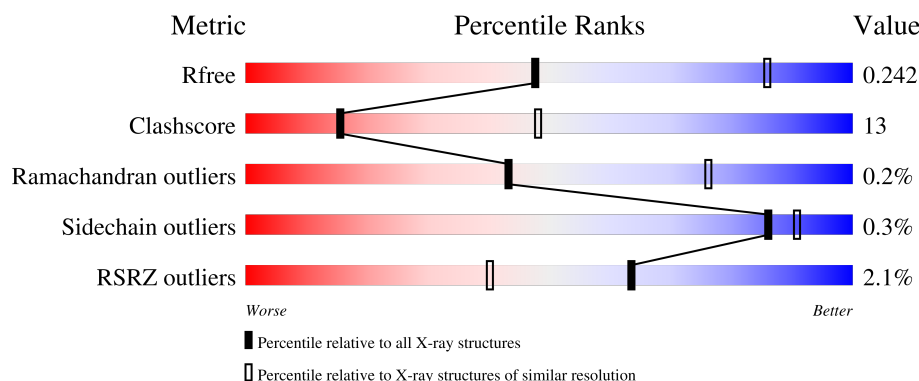
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

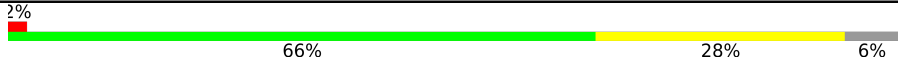
The reported resolution of this entry is 3.00 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	705	
1	B	705	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10546 atoms, of which 16 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5237	3326	906	979	26			
1	B	662	Total	C	N	O	S	0	0	0
			5239	3326	908	979	26			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP Q6A562
A	-29	SER	-	expression tag	UNP Q6A562
A	-28	TYR	-	expression tag	UNP Q6A562
A	-27	TYR	-	expression tag	UNP Q6A562
A	-26	HIS	-	expression tag	UNP Q6A562
A	-25	HIS	-	expression tag	UNP Q6A562
A	-24	HIS	-	expression tag	UNP Q6A562
A	-23	HIS	-	expression tag	UNP Q6A562
A	-22	HIS	-	expression tag	UNP Q6A562
A	-21	HIS	-	expression tag	UNP Q6A562
A	-20	ASP	-	expression tag	UNP Q6A562
A	-19	TYR	-	expression tag	UNP Q6A562
A	-18	ASP	-	expression tag	UNP Q6A562
A	-17	ILE	-	expression tag	UNP Q6A562
A	-16	PRO	-	expression tag	UNP Q6A562
A	-15	THR	-	expression tag	UNP Q6A562
A	-14	THR	-	expression tag	UNP Q6A562
A	-13	GLU	-	expression tag	UNP Q6A562
A	-12	ASN	-	expression tag	UNP Q6A562
A	-11	LEU	-	expression tag	UNP Q6A562
A	-10	TYR	-	expression tag	UNP Q6A562
A	-9	PHE	-	expression tag	UNP Q6A562
A	-8	GLN	-	expression tag	UNP Q6A562
A	-7	GLY	-	expression tag	UNP Q6A562
A	-6	ALA	-	expression tag	UNP Q6A562

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q6A562
A	-4	GLY	-	expression tag	UNP Q6A562
A	-3	ALA	-	expression tag	UNP Q6A562
A	-2	MET	-	expression tag	UNP Q6A562
A	-1	GLY	-	expression tag	UNP Q6A562
A	0	ILE	-	expression tag	UNP Q6A562
B	-30	MET	-	initiating methionine	UNP Q6A562
B	-29	SER	-	expression tag	UNP Q6A562
B	-28	TYR	-	expression tag	UNP Q6A562
B	-27	TYR	-	expression tag	UNP Q6A562
B	-26	HIS	-	expression tag	UNP Q6A562
B	-25	HIS	-	expression tag	UNP Q6A562
B	-24	HIS	-	expression tag	UNP Q6A562
B	-23	HIS	-	expression tag	UNP Q6A562
B	-22	HIS	-	expression tag	UNP Q6A562
B	-21	HIS	-	expression tag	UNP Q6A562
B	-20	ASP	-	expression tag	UNP Q6A562
B	-19	TYR	-	expression tag	UNP Q6A562
B	-18	ASP	-	expression tag	UNP Q6A562
B	-17	ILE	-	expression tag	UNP Q6A562
B	-16	PRO	-	expression tag	UNP Q6A562
B	-15	THR	-	expression tag	UNP Q6A562
B	-14	THR	-	expression tag	UNP Q6A562
B	-13	GLU	-	expression tag	UNP Q6A562
B	-12	ASN	-	expression tag	UNP Q6A562
B	-11	LEU	-	expression tag	UNP Q6A562
B	-10	TYR	-	expression tag	UNP Q6A562
B	-9	PHE	-	expression tag	UNP Q6A562
B	-8	GLN	-	expression tag	UNP Q6A562
B	-7	GLY	-	expression tag	UNP Q6A562
B	-6	ALA	-	expression tag	UNP Q6A562
B	-5	MET	-	expression tag	UNP Q6A562
B	-4	GLY	-	expression tag	UNP Q6A562
B	-3	ALA	-	expression tag	UNP Q6A562
B	-2	MET	-	expression tag	UNP Q6A562
B	-1	GLY	-	expression tag	UNP Q6A562
B	0	ILE	-	expression tag	UNP Q6A562

- Molecule 2 is LUTETIUM (III) ION (CCD ID: LU) (formula: Lu).

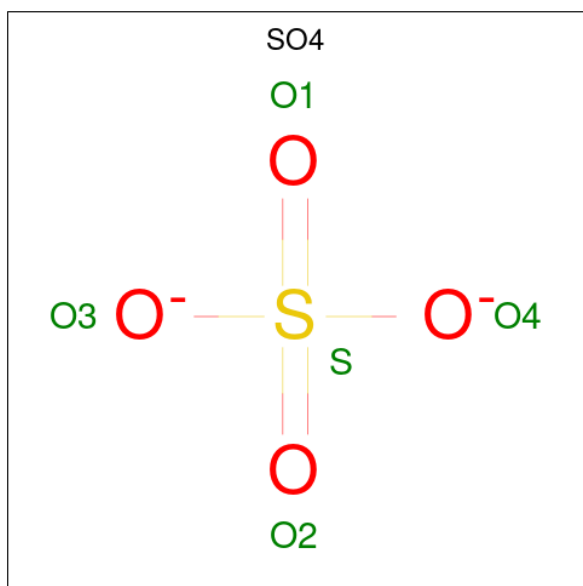
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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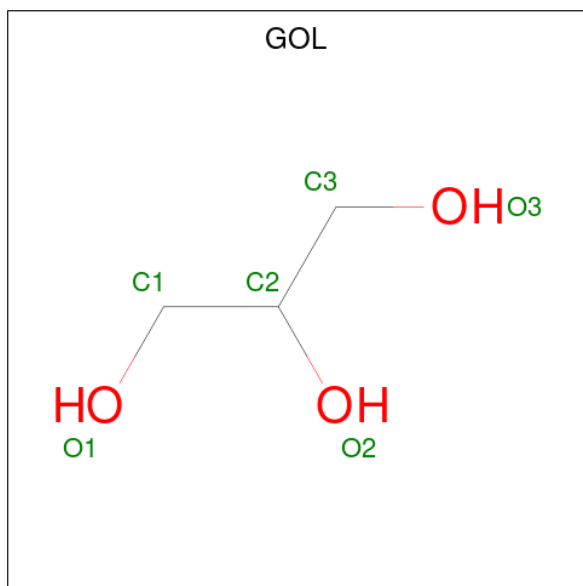
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Lu 1 1	0	0
2	B	1	Total Lu 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

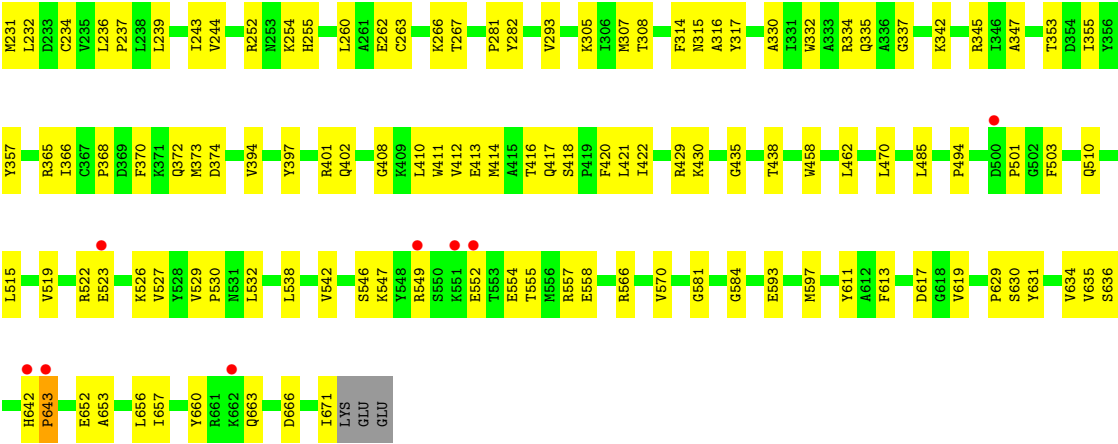


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.05Å 224.57Å 128.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.52 – 3.00 63.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (63.52-3.00) 98.5 (63.52-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.182 , 0.244 0.186 , 0.242	Depositor DCC
R_{free} test set	2230 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10546	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, GOL, LU

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	0.27	0/5356	0.68	0/7255
1	B	0.27	0/5359	0.69	2/7259 (0.0%)
All	All	0.27	0/10715	0.68	2/14514 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	TYR	CA-C-N	5.36	125.07	119.82
1	B	397	TYR	C-N-CA	5.36	125.07	119.82

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	5237	0	5195	167	0
1	B	5239	0	5196	126	0
2	A	1	0	0	0	1
2	B	1	0	0	0	1
3	A	20	0	0	0	0
3	B	20	0	0	1	0
4	A	12	16	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10530	16	10407	280	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 13.

All (280) 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:293:VAL:HG11	1:B:414:MET:HE1	1.49	0.93
1:A:636:SER:HB2	1:A:643:PRO:HA	1.52	0.89
1:B:394:VAL:HG11	1:B:401:ARG:HG3	1.55	0.89
1:B:522:ARG:HH21	1:B:643:PRO:HD2	1.41	0.85
1:B:411:TRP:HA	1:B:414:MET:HE2	1.61	0.82
1:A:24:MET:HE2	1:A:24:MET:HA	1.63	0.80
1:B:430:LYS:NZ	1:B:435:GLY:O	2.15	0.80
1:A:260:LEU:HD21	1:A:421:LEU:HD13	1.65	0.78
1:A:553:THR:HG22	1:A:556:MET:HG3	1.65	0.78
1:B:126:VAL:HG13	1:B:127:ASN:H	1.47	0.78
1:B:307:MET:HE2	1:B:316:ALA:HA	1.62	0.78
1:A:68:LEU:HD13	1:A:152:THR:HG22	1.64	0.78
1:A:566:ARG:HH21	1:A:646:MET:HE1	1.49	0.78
1:A:68:LEU:HB3	1:A:152:THR:HG21	1.67	0.75
1:A:18:MET:HE2	1:B:212:ALA:HB2	1.68	0.74
1:A:286:PRO:HG2	1:A:289:LEU:HD12	1.68	0.74
1:B:33:LEU:HD11	1:B:657:ILE:HD12	1.69	0.73
1:B:236:LEU:HB3	1:B:237:PRO:HD3	1.70	0.72
1:A:562:PHE:CE2	1:A:566:ARG:HD2	2.23	0.72
1:A:293:VAL:HG11	1:A:414:MET:HE1	1.72	0.71
1:A:307:MET:CE	1:A:316:ALA:HA	2.20	0.71
1:B:307:MET:CE	1:B:316:ALA:HA	2.20	0.71
1:A:337:GLY:HA3	1:A:342:LYS:HB2	1.73	0.70
1:A:228:LEU:HB3	1:A:229:PRO:HD3	1.74	0.70
1:A:83:LEU:HD13	1:A:422:ILE:HD12	1.74	0.69
1:B:411:TRP:HA	1:B:414:MET:CE	2.23	0.69
1:A:373:MET:HE1	1:A:451:SER:HB2	1.76	0.68
1:A:430:LYS:NZ	1:A:435:GLY:O	2.25	0.68
1:B:168:GLN:HB3	1:B:372:GLN:NE2	2.09	0.68
1:B:254:LYS:HD2	1:B:255:HIS:NE2	2.08	0.68
1:A:553:THR:CG2	1:A:556:MET:HG3	2.24	0.67
1:A:236:LEU:HB3	1:A:237:PRO:HD3	1.75	0.67
1:B:293:VAL:HG11	1:B:414:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:PRO:HB2	1:B:519:VAL:HG21	1.77	0.67
1:A:415:ALA:HA	1:A:440:VAL:HG21	1.76	0.67
1:A:285:HIS:CE1	1:A:440:VAL:HG22	2.30	0.67
1:A:472:GLU:HG3	1:A:492:TRP:HB3	1.78	0.66
1:A:671:ILE:HG12	1:B:402:GLN:HB3	1.77	0.66
1:A:242:HIS:CD2	1:A:251:LEU:HB2	2.32	0.65
1:A:126:VAL:HG23	1:A:127:ASN:H	1.62	0.65
1:A:611:TYR:CE2	1:A:613:PHE:HB2	2.31	0.65
1:A:255:HIS:HB3	1:A:258:LEU:HD13	1.79	0.64
1:A:332:TRP:CE2	1:A:345:ARG:HD2	2.33	0.64
1:B:33:LEU:CD1	1:B:657:ILE:HD12	2.27	0.64
1:B:123:ALA:HB3	1:B:547:LYS:NZ	2.13	0.64
1:A:249:THR:O	1:A:253:ASN:ND2	2.29	0.63
1:B:228:LEU:HB3	1:B:229:PRO:HD3	1.79	0.63
1:B:416:THR:O	1:B:430:LYS:HE2	1.98	0.63
1:B:522:ARG:NH2	1:B:643:PRO:HD2	2.12	0.62
1:A:307:MET:HE1	1:A:316:ALA:HA	1.81	0.62
1:A:307:MET:HG2	1:A:308:THR:N	2.13	0.62
1:A:653:ALA:O	1:A:657:ILE:HG12	1.99	0.62
1:B:501:PRO:HB2	1:B:519:VAL:CG2	2.30	0.62
1:A:68:LEU:HD13	1:A:152:THR:CG2	2.29	0.62
1:A:371:LYS:CE	1:A:488:LYS:HG3	2.31	0.61
1:A:286:PRO:HB2	1:A:288:HIS:CE1	2.35	0.61
1:A:671:ILE:HD12	1:B:244:VAL:HA	1.83	0.61
1:B:642:HIS:N	1:B:643:PRO:HD3	2.16	0.61
1:A:260:LEU:HD11	1:A:421:LEU:HD13	1.81	0.60
1:B:254:LYS:HD2	1:B:255:HIS:CD2	2.36	0.60
1:B:230:ASP:O	1:B:234:CYS:HB3	2.01	0.60
1:A:260:LEU:HD11	1:A:421:LEU:CD1	2.30	0.60
1:A:125:GLY:O	1:A:547:LYS:NZ	2.36	0.59
1:A:210:THR:HA	1:B:10:PRO:O	2.03	0.59
1:B:653:ALA:O	1:B:657:ILE:HG12	2.03	0.59
1:A:421:LEU:HD11	1:A:427:VAL:HG22	1.84	0.58
1:A:163:GLN:O	1:A:167:MET:HG3	2.02	0.58
1:A:371:LYS:HD2	1:A:486:VAL:HG11	1.85	0.58
1:B:611:TYR:CE2	1:B:613:PHE:HB2	2.39	0.58
1:A:24:MET:SD	1:A:598:ARG:NH1	2.73	0.58
1:B:307:MET:HG2	1:B:308:THR:N	2.16	0.58
1:B:366:ILE:HG22	1:B:368:PRO:HD3	1.86	0.57
1:B:394:VAL:CG1	1:B:401:ARG:HG3	2.32	0.57
1:B:617:ASP:OD2	1:B:619:VAL:HB	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:MET:HA	1:B:418:SER:OG	2.04	0.57
1:A:260:LEU:HD21	1:A:421:LEU:CD1	2.34	0.57
1:A:371:LYS:HE2	1:A:488:LYS:HG3	1.87	0.57
1:B:316:ALA:HB2	1:B:347:ALA:HB1	1.85	0.57
1:B:161:PHE:CE1	1:B:281:PRO:HB3	2.40	0.57
1:B:186:LEU:HD22	1:B:314:PHE:CD1	2.39	0.57
1:A:209:LYS:HA	1:B:14:SER:HA	1.87	0.56
1:B:168:GLN:HB3	1:B:372:GLN:HE21	1.69	0.56
1:A:328:ASP:OD1	1:A:640:ARG:NH2	2.36	0.56
1:A:371:LYS:HE3	1:A:488:LYS:HA	1.87	0.56
1:A:68:LEU:HD22	1:A:152:THR:CG2	2.35	0.55
1:A:240:TYR:OH	1:B:666:ASP:O	2.21	0.55
1:A:449:VAL:O	1:A:453:LEU:HG	2.07	0.55
1:B:365:ARG:O	1:B:494:PRO:HA	2.05	0.55
1:A:357:TYR:HE2	1:A:366:ILE:HD11	1.72	0.54
1:A:374:ASP:OD2	1:A:438:THR:OG1	2.22	0.54
1:A:630:SER:HB2	4:A:705:GOL:H31	1.89	0.54
1:A:414:MET:HA	1:A:418:SER:HB2	1.89	0.54
1:A:636:SER:CB	1:A:643:PRO:HA	2.30	0.54
1:A:307:MET:HG2	1:A:308:THR:HG23	1.90	0.54
1:A:411:TRP:HA	1:A:414:MET:HE2	1.91	0.53
1:A:20:ALA:O	1:A:24:MET:HG2	2.08	0.53
1:B:83:LEU:HD13	1:B:422:ILE:HD12	1.89	0.53
1:A:293:VAL:HG11	1:A:414:MET:CE	2.37	0.53
1:A:525:GLU:OE1	1:A:525:GLU:N	2.42	0.53
1:B:98:LEU:HD23	1:B:103:PRO:HA	1.90	0.53
1:B:307:MET:HG2	1:B:308:THR:HG23	1.90	0.53
1:A:239:LEU:O	1:A:243:ILE:HG13	2.08	0.53
1:A:529:VAL:HB	1:A:530:PRO:HD2	1.90	0.53
1:A:605:ARG:HD3	1:A:622:PHE:O	2.08	0.53
1:B:260:LEU:HD21	1:B:421:LEU:HG	1.91	0.53
1:A:353:THR:HG22	1:A:355:ILE:CD1	2.39	0.52
1:A:437:MET:O	1:A:440:VAL:HG23	2.10	0.52
1:B:118:VAL:HG21	1:B:262:GLU:OE2	2.09	0.52
1:A:186:LEU:HD22	1:A:314:PHE:CD1	2.44	0.51
1:A:285:HIS:HB3	1:A:286:PRO:HD2	1.91	0.51
1:B:293:VAL:CG1	1:B:414:MET:HE1	2.30	0.51
1:B:140:ASP:O	1:B:144:VAL:HG23	2.10	0.51
1:A:593:GLU:O	1:A:597:MET:HB2	2.10	0.51
1:A:209:LYS:HG2	1:B:14:SER:HB3	1.93	0.50
1:A:457:ASP:O	1:A:461:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ARG:NH2	3:B:705:SO4:O2	2.44	0.50
1:A:196:ASP:HA	1:A:397:TYR:CE2	2.46	0.50
1:A:559:ARG:HD3	1:A:597:MET:HE2	1.93	0.50
1:A:216:ALA:HB1	1:A:287:PHE:HB2	1.93	0.50
1:A:153:TYR:CD1	1:A:545:ARG:HA	2.46	0.50
1:B:266:LYS:HB2	1:B:282:TYR:CD1	2.48	0.49
1:B:239:LEU:O	1:B:243:ILE:HG13	2.11	0.49
1:A:68:LEU:HD22	1:A:152:THR:HG23	1.94	0.49
1:B:552:GLU:HG2	1:B:557:ARG:HG3	1.94	0.49
1:A:371:LYS:HE3	1:A:488:LYS:HG3	1.94	0.49
1:B:394:VAL:HG22	1:B:401:ARG:HA	1.95	0.49
1:A:381:THR:O	1:A:385:VAL:HG23	2.12	0.49
1:A:13:LEU:HD11	1:A:18:MET:HG2	1.93	0.48
1:A:553:THR:HG22	1:A:556:MET:CG	2.41	0.48
1:A:353:THR:HG22	1:A:355:ILE:HD11	1.95	0.48
1:A:85:PHE:O	1:A:431:MET:HE2	2.14	0.48
1:A:307:MET:HE2	1:A:315:ASN:O	2.14	0.48
1:B:142:ASP:OD1	1:B:143:LEU:N	2.46	0.48
1:A:218:PRO:HB2	1:A:257:GLU:HG2	1.94	0.48
1:B:408:GLY:O	1:B:412:VAL:HG23	2.13	0.48
1:B:126:VAL:HG22	1:B:127:ASN:ND2	2.29	0.48
1:A:194:LEU:HD22	1:A:393:HIS:NE2	2.28	0.48
1:A:205:VAL:O	1:B:15:LEU:HD12	2.12	0.48
1:A:631:TYR:O	1:A:635:VAL:HG23	2.13	0.48
1:A:212:ALA:HB1	1:A:225:ARG:HB2	1.96	0.48
1:A:337:GLY:HA3	1:A:342:LYS:CB	2.43	0.47
1:A:472:GLU:CG	1:A:492:TRP:HB3	2.44	0.47
1:B:126:VAL:HG22	1:B:127:ASN:N	2.29	0.47
1:A:252:ARG:NH2	1:A:413:GLU:OE1	2.47	0.47
1:A:285:HIS:CD2	1:A:414:MET:HB3	2.49	0.47
1:B:315:ASN:OD1	1:B:317:TYR:HB3	2.15	0.47
1:B:410:LEU:O	1:B:414:MET:HG3	2.14	0.47
1:A:394:VAL:HG11	1:A:401:ARG:HG3	1.96	0.47
1:A:286:PRO:CG	1:A:289:LEU:HD12	2.39	0.47
1:A:532:LEU:HB2	1:A:537:TRP:CE2	2.50	0.47
1:B:200:GLU:OE1	1:B:202:SER:HB2	2.15	0.47
1:B:593:GLU:O	1:B:597:MET:HB3	2.15	0.47
1:A:33:LEU:HD11	1:A:657:ILE:HD12	1.97	0.47
1:B:186:LEU:HD22	1:B:314:PHE:CE1	2.49	0.47
1:B:252:ARG:NH2	1:B:413:GLU:OE1	2.47	0.47
1:B:366:ILE:HG12	1:B:494:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:SER:HB2	1:B:642:HIS:HA	1.95	0.47
1:A:23:ALA:O	1:A:27:ARG:HG3	2.15	0.47
1:A:54:ARG:CB	1:A:137:ARG:HH12	2.27	0.47
1:B:337:GLY:HA3	1:B:342:LYS:HB2	1.96	0.47
1:A:304:LEU:O	1:A:616:ARG:NH2	2.46	0.47
1:B:546:SER:HB2	1:B:549:ARG:NH2	2.30	0.47
1:A:54:ARG:HA	1:A:137:ARG:NH1	2.31	0.46
1:B:46:PRO:O	1:B:584:GLY:HA3	2.15	0.46
1:B:522:ARG:HB2	1:B:527:VAL:CG2	2.46	0.46
1:B:566:ARG:HA	1:B:629:PRO:HG2	1.98	0.46
1:B:212:ALA:HB1	1:B:225:ARG:HB2	1.97	0.46
1:B:374:ASP:OD2	1:B:438:THR:OG1	2.23	0.46
1:A:98:LEU:HA	1:A:103:PRO:HA	1.97	0.46
1:B:30:LEU:HD11	1:B:555:THR:HG21	1.97	0.46
1:B:335:GLN:HB2	1:B:345:ARG:HE	1.80	0.46
1:B:357:TYR:CE2	1:B:470:LEU:HD13	2.51	0.46
1:A:72:VAL:O	1:A:76:GLN:HG3	2.17	0.45
1:A:307:MET:HE2	1:A:316:ALA:HA	1.97	0.45
1:A:538:LEU:O	1:A:542:VAL:HG22	2.17	0.45
1:B:260:LEU:HD21	1:B:421:LEU:CD1	2.47	0.45
1:A:65:THR:HG21	1:A:129:SER:OG	2.16	0.45
1:A:218:PRO:HB3	1:A:221:TRP:CZ2	2.51	0.45
1:B:123:ALA:HB3	1:B:547:LYS:HZ1	1.78	0.45
1:B:554:GLU:O	1:B:558:GLU:HG3	2.16	0.45
1:A:394:VAL:HG13	1:A:401:ARG:HB2	1.98	0.45
1:A:120:ARG:HG3	1:A:122:PHE:CE2	2.52	0.45
1:A:365:ARG:HB2	1:A:497:VAL:CG2	2.46	0.45
1:A:665:MET:HB2	1:B:201:LEU:HB3	1.99	0.45
1:A:355:ILE:HB	1:A:366:ILE:HB	1.99	0.45
1:B:120:ARG:HA	1:B:120:ARG:NH1	2.32	0.45
1:A:174:VAL:HG11	1:A:482:LYS:O	2.17	0.45
1:A:233:ASP:HB2	1:B:660:TYR:HB2	1.99	0.45
1:A:503:PHE:CE1	1:A:526:LYS:HG2	2.52	0.45
1:B:355:ILE:N	1:B:355:ILE:HD12	2.31	0.45
1:A:13:LEU:HD11	1:A:18:MET:CG	2.47	0.45
1:A:197:VAL:HA	1:A:204:LEU:HD11	1.98	0.45
1:A:371:LYS:HD2	1:A:486:VAL:CG1	2.46	0.45
1:B:218:PRO:HG3	1:B:221:TRP:CZ2	2.52	0.45
1:A:268:ASP:OD1	1:A:269:ARG:N	2.44	0.44
1:A:553:THR:HG23	1:A:556:MET:H	1.82	0.44
1:A:75:ALA:HB1	1:A:157:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:CYS:SG	1:A:97:ILE:HG13	2.57	0.44
1:B:126:VAL:HG13	1:B:127:ASN:N	2.24	0.44
1:A:330:ALA:O	1:A:334:ARG:HG3	2.16	0.44
1:B:305:LYS:HE2	1:B:305:LYS:HA	1.99	0.44
1:B:566:ARG:O	1:B:570:VAL:HG23	2.17	0.44
1:A:33:LEU:CD1	1:A:657:ILE:HD12	2.47	0.44
1:A:327:GLU:O	1:A:331:ILE:HG13	2.17	0.44
1:B:630:SER:O	1:B:634:VAL:HG23	2.18	0.44
1:B:330:ALA:O	1:B:334:ARG:HG3	2.18	0.44
1:B:370:PHE:CZ	1:B:485:LEU:HD13	2.53	0.44
1:B:139:GLU:HG3	1:B:140:ASP:N	2.33	0.44
1:B:353:THR:HG22	1:B:355:ILE:CD1	2.48	0.44
1:A:332:TRP:NE1	1:A:345:ARG:HD2	2.33	0.44
1:A:371:LYS:C	1:A:372:GLN:HG2	2.43	0.44
1:B:566:ARG:HG2	1:B:629:PRO:HD3	2.00	0.44
1:A:56:SER:O	1:A:60:GLN:HG3	2.18	0.43
1:A:246:LYS:HG3	1:B:671:ILE:CG2	2.47	0.43
1:A:627:GLY:C	1:A:646:MET:HE2	2.43	0.43
1:B:218:PRO:HG3	1:B:221:TRP:CH2	2.53	0.43
1:A:633:TRP:CH2	1:A:637:LEU:HD11	2.53	0.43
1:A:671:ILE:CD1	1:B:244:VAL:HA	2.47	0.43
1:B:652:GLU:O	1:B:656:LEU:HD13	2.18	0.43
1:B:75:ALA:HB1	1:B:157:THR:HG21	2.00	0.43
1:A:80:HIS:CD2	1:A:158:TRP:HB3	2.54	0.43
1:A:87:GLU:CD	1:A:429:ARG:HH21	2.26	0.43
1:A:171:ARG:HH21	1:A:372:GLN:HG3	1.84	0.43
1:A:218:PRO:O	1:A:286:PRO:HB3	2.19	0.43
1:A:357:TYR:CE2	1:A:366:ILE:HD11	2.53	0.43
1:B:515:LEU:HD23	1:B:532:LEU:HD11	2.01	0.43
1:B:522:ARG:HB2	1:B:527:VAL:HG23	2.01	0.43
1:B:529:VAL:HB	1:B:530:PRO:HD2	2.01	0.43
1:A:237:PRO:HB3	1:B:663:GLN:NE2	2.34	0.42
1:A:411:TRP:HA	1:A:414:MET:CE	2.49	0.42
1:B:263:CYS:HB2	1:B:420:PHE:CD2	2.54	0.42
1:A:293:VAL:CG1	1:A:414:MET:HE1	2.45	0.42
1:A:355:ILE:HD12	1:A:355:ILE:N	2.34	0.42
1:B:522:ARG:O	1:B:523:GLU:HG2	2.19	0.42
1:A:507:TRP:HB3	1:A:517:LEU:HB3	2.01	0.42
1:A:650:PHE:HA	1:A:651:PRO:HD2	1.93	0.42
1:B:332:TRP:NE1	1:B:345:ARG:HD2	2.34	0.42
1:A:13:LEU:CD1	1:A:18:MET:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HD3	1:A:164:ARG:HA	1.83	0.42
1:B:47:GLN:HA	1:B:581:GLY:HA2	2.00	0.42
1:A:385:VAL:HG22	1:A:449:VAL:HG11	2.02	0.42
1:A:527:VAL:HG11	1:A:635:VAL:HG13	2.02	0.42
1:A:628:TYR:HA	1:A:629:PRO:HD3	1.89	0.42
1:A:358:ARG:HA	1:A:362:LYS:O	2.20	0.42
1:B:67:GLU:OE1	1:B:145:ARG:NH2	2.51	0.42
1:B:365:ARG:HD3	1:B:510:GLN:OE1	2.20	0.42
1:A:206:LEU:HD21	1:A:232:LEU:HD22	2.02	0.41
1:A:634:VAL:O	1:A:637:LEU:HB2	2.20	0.41
1:A:24:MET:HE2	1:A:24:MET:CA	2.43	0.41
1:A:260:LEU:O	1:A:286:PRO:HD3	2.20	0.41
1:A:368:PRO:HG2	1:A:455:TYR:OH	2.20	0.41
1:A:410:LEU:O	1:A:414:MET:HG3	2.20	0.41
1:A:128:THR:O	1:A:129:SER:HB2	2.19	0.41
1:B:631:TYR:O	1:B:635:VAL:HG23	2.21	0.41
1:A:69:LYS:HE2	1:A:69:LYS:HB3	1.81	0.41
1:B:366:ILE:HG22	1:B:368:PRO:HG3	2.03	0.41
1:B:102:HIS:NE2	1:B:230:ASP:OD2	2.47	0.41
1:B:355:ILE:HB	1:B:366:ILE:HB	2.03	0.41
1:B:206:LEU:HD21	1:B:232:LEU:HD21	2.03	0.41
1:A:24:MET:HA	1:A:24:MET:CE	2.44	0.41
1:A:316:ALA:HB3	1:A:349:TYR:HB2	2.03	0.41
1:B:370:PHE:HB3	1:B:373:MET:HB3	2.01	0.41
1:B:538:LEU:O	1:B:542:VAL:HG22	2.19	0.41
1:A:104:VAL:O	1:A:106:PRO:HD3	2.21	0.41
1:A:591:ALA:HA	1:A:592:PRO:HD3	1.97	0.41
1:B:105:HIS:HA	1:B:106:PRO:HD2	1.89	0.41
1:A:286:PRO:HG2	1:A:289:LEU:CD1	2.46	0.40
1:A:289:LEU:HB3	1:A:414:MET:SD	2.61	0.40
1:A:602:GLY:HA3	1:A:606:GLY:O	2.21	0.40
1:B:56:SER:O	1:B:60:GLN:HG3	2.21	0.40
1:B:307:MET:CG	1:B:308:THR:HG23	2.51	0.40
1:B:417:GLN:HG3	1:B:429:ARG:HD2	2.02	0.40
1:B:98:LEU:HD23	1:B:103:PRO:CA	2.51	0.40
1:A:13:LEU:C	1:A:13:LEU:HD12	2.47	0.40
1:A:194:LEU:HD22	1:A:393:HIS:HE2	1.86	0.40
1:B:366:ILE:HG22	1:B:368:PRO:CD	2.51	0.40
1:A:218:PRO:HG2	1:A:260:LEU:O	2.21	0.40
1:B:458:TRP:CH2	1:B:462:LEU:HD11	2.55	0.40
1:B:503:PHE:CE1	1:B:526:LYS:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:TYR:CZ	1:B:267:THR:HG22	2.57	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)
2:A:701:LU:LU	2:B:701:LU:LU[8_556]	1.59	0.61

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	661/705 (94%)	624 (94%)	37 (6%)	0	100	100
1	B	660/705 (94%)	626 (95%)	32 (5%)	2 (0%)	36	70
All	All	1321/1410 (94%)	1250 (95%)	69 (5%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	ARG
1	B	643	PRO

5.3.2 Protein sidechains [i](#)

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	560/598 (94%)	559 (100%)	1 (0%)	87	92
1	B	561/598 (94%)	559 (100%)	2 (0%)	84	90
All	All	1121/1196 (94%)	1118 (100%)	3 (0%)	86	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	MET
1	B	120	ARG
1	B	231	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	B	28	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	SO4	B	703	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	702	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	704	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	707	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	703	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	702	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	A	706	-	5,5,5	0.34	0	5,5,5	0.30	0
3	SO4	A	704	-	4,4,4	0.23	0	6,6,6	0.07	0
4	GOL	A	705	-	5,5,5	0.39	0	5,5,5	0.27	0
3	SO4	B	705	-	4,4,4	0.24	0	6,6,6	0.08	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
4	GOL	A	706	-	-	3/4/4/4	-
4	GOL	A	705	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	GOL	O1-C1-C2-C3
4	A	705	GOL	O1-C1-C2-O2
4	A	706	GOL	O1-C1-C2-O2
4	A	706	GOL	O2-C2-C3-O3
4	A	706	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	705	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	663/705 (94%)	-0.19	11 (1%) 69 45	13, 34, 63, 88	0
1	B	662/705 (93%)	-0.37	17 (2%) 57 34	9, 25, 60, 91	0
All	All	1325/1410 (93%)	-0.28	28 (2%) 63 40	9, 30, 62, 91	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	PRO	6.9
1	B	11	THR	5.8
1	B	140	ASP	5.3
1	A	10	PRO	4.2
1	A	11	THR	4.1
1	A	127	ASN	4.0
1	A	140	ASP	3.9
1	A	642	HIS	3.6
1	A	551	LYS	3.4
1	B	643	PRO	3.4
1	B	500	ASP	3.4
1	B	142	ASP	3.2
1	B	128	THR	3.2
1	A	672	LYS	2.8
1	B	662	LYS	2.6
1	A	662	LYS	2.6
1	B	549	ARG	2.5
1	B	642	HIS	2.4
1	B	127	ASN	2.3
1	B	12	ARG	2.3
1	B	126	VAL	2.3
1	A	669	VAL	2.1
1	A	641	ASP	2.1
1	B	523	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	552	GLU	2.1
1	B	125	GLY	2.1
1	B	551	LYS	2.0
1	A	99	HIS	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
4	GOL	A	706	6/6	0.61	0.30	63,79,97,105	0
4	GOL	A	705	6/6	0.81	0.23	44,67,86,88	0
3	SO4	A	707	5/5	0.81	0.21	83,90,94,96	0
3	SO4	B	705	5/5	0.86	0.17	70,72,78,84	0
3	SO4	B	704	5/5	0.95	0.09	41,43,56,63	0
3	SO4	A	702	5/5	0.96	0.09	37,40,58,65	0
3	SO4	A	703	5/5	0.97	0.10	24,37,45,49	0
2	LU	A	701	1/1	0.97	0.23	232,232,232,232	0
3	SO4	A	704	5/5	0.98	0.08	39,52,54,57	0
2	LU	B	701	1/1	0.98	0.11	103,103,103,103	0
3	SO4	B	702	5/5	0.98	0.08	24,35,47,51	0
3	SO4	B	703	5/5	0.98	0.07	17,37,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.