



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:36 PM EDT

PDB ID : 4ON9 / pdb_00004on9
Title : DECH box helicase domain
Authors : Deimling, T.; Witte, G.; Hopfner, K.P.
Deposited on : 2014-01-28
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

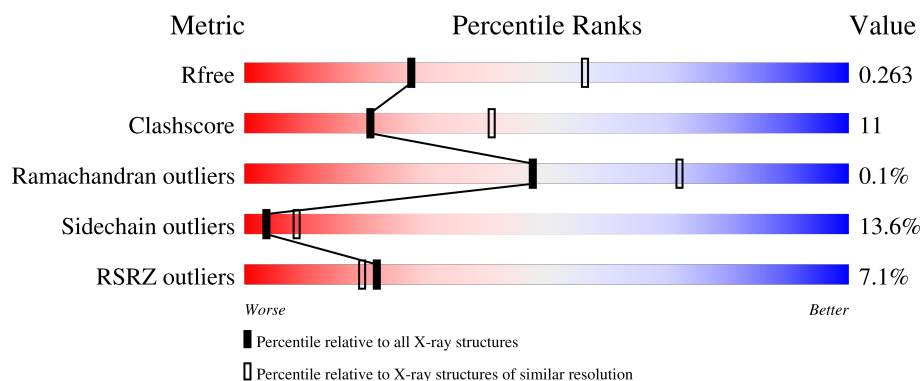
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	580	5% 64% 21% • 11%
1	B	580	7% 54% 27% • 15%

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	SO4	A	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8183 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	60	0	0
			4130	2641	695	771	23			
1	B	495	Total	C	N	O	S	73	0	0
			3996	2557	673	743	23			

There are 32 discrepancies between the modelled and reference sequences:

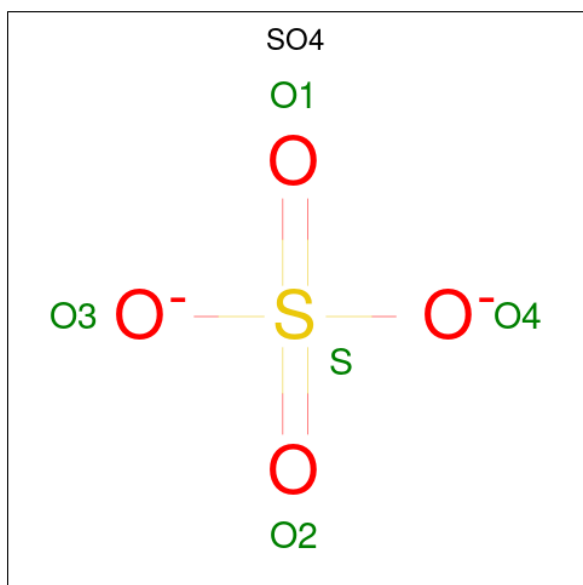
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	expression tag	UNP O95786
A	215	GLY	-	expression tag	UNP O95786
A	216	SER	-	expression tag	UNP O95786
A	217	SER	-	expression tag	UNP O95786
A	218	HIS	-	expression tag	UNP O95786
A	219	HIS	-	expression tag	UNP O95786
A	220	HIS	-	expression tag	UNP O95786
A	221	HIS	-	expression tag	UNP O95786
A	222	HIS	-	expression tag	UNP O95786
A	223	HIS	-	expression tag	UNP O95786
A	224	SER	-	expression tag	UNP O95786
A	225	GLN	-	expression tag	UNP O95786
A	226	ASP	-	expression tag	UNP O95786
A	227	PRO	-	expression tag	UNP O95786
A	228	ASN	-	expression tag	UNP O95786
A	229	SER	-	expression tag	UNP O95786
B	214	MET	-	expression tag	UNP O95786
B	215	GLY	-	expression tag	UNP O95786
B	216	SER	-	expression tag	UNP O95786
B	217	SER	-	expression tag	UNP O95786
B	218	HIS	-	expression tag	UNP O95786
B	219	HIS	-	expression tag	UNP O95786
B	220	HIS	-	expression tag	UNP O95786
B	221	HIS	-	expression tag	UNP O95786
B	222	HIS	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	223	HIS	-	expression tag	UNP O95786
B	224	SER	-	expression tag	UNP O95786
B	225	GLN	-	expression tag	UNP O95786
B	226	ASP	-	expression tag	UNP O95786
B	227	PRO	-	expression tag	UNP O95786
B	228	ASN	-	expression tag	UNP O95786
B	229	SER	-	expression tag	UNP O95786

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



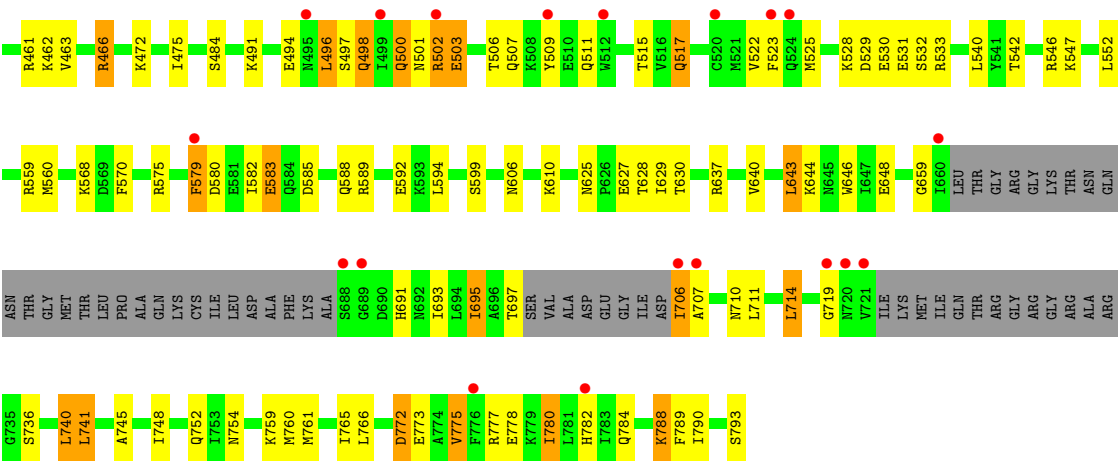
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	18	Total 18	O 18	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.91Å 112.99Å 124.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.71 49.06 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.06-2.71) 99.2 (49.06-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.219 , 0.258 0.223 , 0.263	Depositor DCC
R_{free} test set	1891 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8183	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, CL

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	0.37	0/4203	0.79	2/5662 (0.0%)
1	B	0.43	0/4067	0.85	1/5478 (0.0%)
All	All	0.40	0/8270	0.82	3/11140 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	775	VAL	N-CA-C	6.17	116.92	110.62
1	A	608	ASN	CA-C-N	5.52	125.18	119.05
1	A	608	ASN	C-N-CA	5.52	125.18	119.05

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	4130	0	4177	83	0
1	B	3996	0	4038	100	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
3	B	1	0	0	1	0
4	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	0	0	1	0
All	All	8183	0	8215	178	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 11.

All (178) 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:466:ARG:HE	1:B:560:MET:HE3	1.33	0.92
1:B:377:THR:HG21	1:B:434:LEU:HD21	1.64	0.79
1:A:685:PHE:CG	1:A:686:LYS:HA	2.19	0.77
1:A:292:LYS:NZ	1:A:341:ASN:O	2.18	0.77
1:B:246:TYR:HB3	1:B:445:ASN:HB2	1.70	0.73
1:B:466:ARG:HH21	1:B:466:ARG:HG3	1.52	0.73
1:A:724:MET:HE1	1:A:738:CYS:HB2	1.70	0.73
1:B:461:ARG:HB2	1:B:741:LEU:HD22	1.71	0.72
1:B:377:THR:HG22	1:B:383:TYR:HB3	1.70	0.71
1:A:397:GLY:HA2	1:A:398:SER:C	2.17	0.69
1:A:258:LYS:NZ	1:A:773:GLU:OE2	2.26	0.69
1:B:466:ARG:NE	1:B:560:MET:HE3	2.06	0.69
1:A:533:ARG:HH11	1:A:533:ARG:HB2	1.59	0.67
1:B:368:LEU:HD13	1:B:404:GLN:HB3	1.75	0.66
1:B:394:LYS:NZ	1:B:435:ASP:OD1	2.28	0.66
1:B:357:LYS:HB3	1:B:359:THR:HG23	1.77	0.66
1:B:714:LEU:HD23	1:B:740:LEU:HD12	1.78	0.65
1:B:525:MET:HG2	1:B:531:GLU:HB2	1.80	0.64
1:A:335:GLU:H	1:A:335:GLU:CD	2.06	0.63
1:A:477:GLN:OE1	1:A:480:ARG:NH1	2.31	0.63
1:B:466:ARG:HH21	1:B:466:ARG:CG	2.12	0.63
1:B:780:ILE:HG22	1:B:784:GLN:HE21	1.63	0.63
1:B:431:CYS:SG	1:B:439:ILE:HD11	2.39	0.63
1:A:685:PHE:CD1	1:A:686:LYS:HA	2.33	0.62
1:B:348:PRO:HB2	1:B:382:PRO:HB2	1.80	0.62
1:A:685:PHE:O	1:A:708:GLN:NE2	2.33	0.62
1:A:702:GLU:HA	1:B:515:THR:HG22	1.82	0.61
1:B:625:ASN:O	1:B:628:THR:HG23	2.00	0.61
1:A:461:ARG:HB2	1:A:741:LEU:HD22	1.83	0.60
1:A:747:VAL:HG12	1:B:501:ASN:HB3	1.83	0.60
1:A:533:ARG:HH11	1:A:533:ARG:CB	2.14	0.60
1:A:500:GLN:HG2	1:B:719:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG11	1:A:449:LEU:HD22	1.82	0.59
1:B:560:MET:HE1	1:B:606:ASN:HB3	1.85	0.59
1:B:284:LYS:HG2	1:B:286:PRO:HD2	1.85	0.58
1:A:758:GLU:O	1:A:762:ASN:ND2	2.36	0.58
1:B:517:GLN:NE2	1:B:542:THR:OG1	2.38	0.57
1:A:303:TYR:CZ	1:A:325:SER:HB2	2.39	0.56
1:A:502:ARG:HD3	1:A:512:TRP:CD2	2.41	0.56
1:B:498:GLN:NE2	1:B:500:GLN:O	2.38	0.56
1:B:525:MET:N	1:B:531:GLU:OE1	2.35	0.56
1:B:659:GLY:HA3	1:B:691:HIS:ND1	2.21	0.56
1:A:264:ALA:O	1:A:270:LYS:HE2	2.05	0.56
1:B:789:PHE:HD1	1:B:790:ILE:HD12	1.71	0.55
1:A:463:VAL:HB	1:A:610:LYS:HG2	1.88	0.55
1:A:502:ARG:HB2	1:A:509:TYR:HD1	1.70	0.55
1:B:628:THR:HG22	1:B:710:ASN:HD21	1.72	0.54
1:B:271:THR:HG21	1:B:306:GLN:CD	2.33	0.54
1:B:354:ASN:HA	1:B:357:LYS:HB2	1.90	0.53
1:B:640:VAL:HG13	1:B:695:ILE:HB	1.90	0.53
1:B:307:LYS:HA	1:B:345:ILE:HG13	1.89	0.53
1:B:273:VAL:O	1:B:277:ILE:HG12	2.08	0.53
1:B:778:GLU:H	1:B:778:GLU:CD	2.16	0.53
1:A:760:MET:O	1:A:764:SER:OG	2.25	0.53
1:A:418:LYS:HE3	1:A:418:LYS:HA	1.91	0.52
1:A:483:GLU:OE2	1:A:502:ARG:NH1	2.42	0.52
1:A:320:ARG:NH1	1:A:340:ASN:O	2.42	0.52
1:B:259:ASN:HB2	1:B:436:ALA:HA	1.91	0.52
1:B:588:GLN:NE2	1:B:592:GLU:OE1	2.43	0.52
1:B:644:LYS:O	1:B:648:GLU:HG3	2.10	0.52
1:B:780:ILE:O	1:B:784:GLN:HG3	2.10	0.52
1:A:333:PRO:HB2	1:A:335:GLU:OE2	2.10	0.52
1:A:258:LYS:O	1:A:404:GLN:NE2	2.38	0.51
1:B:254:ALA:HB3	1:B:277:ILE:HD12	1.91	0.51
1:B:264:ALA:O	1:B:270:LYS:HE2	2.10	0.51
1:A:255:MET:HE2	1:A:280:HIS:HB2	1.93	0.51
1:B:250:LEU:HD22	1:B:262:ILE:HG23	1.93	0.51
1:B:630:THR:HB	1:B:693:ILE:HG13	1.92	0.51
1:B:279:GLU:HG3	1:B:280:HIS:N	2.26	0.51
1:A:349:GLN:O	1:A:349:GLN:NE2	2.45	0.50
1:A:600:VAL:O	1:A:606:ASN:ND2	2.42	0.50
1:B:443:LYS:HA	1:B:446:LEU:HD12	1.94	0.50
1:B:325:SER:C	1:B:350:ILE:HD11	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:CYS:O	1:B:377:THR:HG23	2.12	0.49
1:A:533:ARG:HH22	1:B:305:GLN:HA	1.76	0.49
1:B:303:TYR:CE2	1:B:325:SER:HB2	2.47	0.49
1:B:559:ARG:HD3	1:B:646:TRP:HD1	1.78	0.49
1:A:334:VAL:HG23	1:A:360:ILE:HD11	1.95	0.49
1:A:510:GLU:O	1:A:514:VAL:HG23	2.13	0.48
1:B:259:ASN:ND2	1:B:435:ASP:O	2.37	0.48
1:A:350:ILE:O	1:A:354:ASN:ND2	2.46	0.48
1:A:502:ARG:HB2	1:A:509:TYR:CD1	2.46	0.48
1:A:772:ASP:OD1	1:A:775:VAL:N	2.32	0.48
1:B:320:ARG:HB2	1:B:341:ASN:HA	1.96	0.48
1:A:588:GLN:HG3	1:A:589:ARG:N	2.28	0.48
1:A:419:ASN:OD1	1:A:420:THR:N	2.46	0.48
1:B:354:ASN:O	1:B:358:GLY:N	2.46	0.48
1:B:580:ASP:OD1	1:B:582:ILE:N	2.46	0.48
1:B:772:ASP:HB2	1:B:775:VAL:HG23	1.96	0.48
1:B:506:THR:HG23	1:B:509:TYR:H	1.79	0.48
1:B:530:GLU:HA	1:B:533:ARG:NH1	2.28	0.48
1:B:745:ALA:O	1:B:748:ILE:HG22	2.13	0.48
1:B:778:GLU:O	1:B:782:HIS:N	2.35	0.48
1:A:429:LYS:O	1:A:433:SER:OG	2.32	0.48
1:B:706:ILE:HG22	1:B:707:ALA:H	1.78	0.47
1:B:710:ASN:HA	1:B:736:SER:HB3	1.95	0.47
1:B:511:GLN:O	1:B:515:THR:HG23	2.14	0.47
1:B:326:GLY:N	1:B:350:ILE:HD11	2.29	0.47
1:B:498:GLN:HE22	1:B:502:ARG:HG3	1.78	0.47
1:A:269:GLY:N	2:A:801:SO4:O3	2.48	0.47
1:A:320:ARG:HD2	1:A:340:ASN:O	2.15	0.47
1:A:335:GLU:HA	1:A:338:VAL:HG12	1.97	0.47
1:A:704:ILE:HG12	1:A:705:ASP:N	2.28	0.47
3:B:803:CL:CL	4:B:918:HOH:O	2.58	0.47
1:A:748:ILE:O	1:A:752:GLN:HG3	2.15	0.46
1:B:585:ASP:OD2	1:B:589:ARG:NH1	2.48	0.46
1:B:364:SER:OG	1:B:401:PRO:O	2.31	0.46
1:A:264:ALA:O	1:A:410:ALA:HA	2.15	0.46
1:B:352:VAL:O	1:B:356:LYS:HG3	2.16	0.46
1:B:263:CYS:HA	1:B:409:THR:O	2.16	0.46
1:A:290:LYS:HE3	1:A:342:ASP:OD1	2.15	0.46
1:B:773:GLU:O	1:B:777:ARG:HG3	2.16	0.46
1:A:598:GLU:O	1:A:602:ARG:HG3	2.16	0.46
1:B:588:GLN:O	1:B:592:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LYS:N	2:A:801:SO4:O3	2.48	0.45
1:A:596:GLU:O	1:A:600:VAL:HG13	2.17	0.45
1:B:580:ASP:HB3	1:B:583:GLU:HB2	1.99	0.45
1:B:439:ILE:HG21	1:B:765:ILE:HD12	2.00	0.45
1:A:571:PHE:O	1:A:575:ARG:HG3	2.16	0.44
1:A:325:SER:C	1:A:350:ILE:HD11	2.42	0.44
1:A:514:VAL:HG22	1:A:546:ARG:HH22	1.82	0.44
1:A:625:ASN:O	1:A:628:THR:OG1	2.27	0.44
1:A:292:LYS:N	1:A:367:THR:OG1	2.44	0.44
1:A:394:LYS:HB2	1:A:402:LEU:CD1	2.47	0.44
1:B:387:MET:HG3	1:B:433:SER:O	2.17	0.44
1:B:463:VAL:HB	1:B:610:LYS:HG2	2.00	0.44
1:B:503:GLU:O	1:B:509:TYR:HB2	2.17	0.44
1:B:579:PHE:HD1	1:B:579:PHE:HA	1.69	0.43
1:A:299:GLN:HB2	1:A:301:PRO:HD2	2.01	0.43
1:B:417:ALA:O	1:B:760:MET:HE1	2.18	0.43
1:A:269:GLY:O	1:A:273:VAL:HG23	2.19	0.43
1:A:580:ASP:HB3	1:A:583:GLU:H	1.82	0.43
1:B:379:LYS:HE2	1:B:379:LYS:HB2	1.76	0.43
1:B:432:ALA:HA	1:B:780:ILE:HG23	2.01	0.43
1:A:320:ARG:NH2	1:A:342:ASP:OD1	2.52	0.43
1:A:398:SER:O	1:A:398:SER:OG	2.30	0.42
1:A:513:ILE:HG21	1:A:546:ARG:HB2	2.01	0.42
1:B:348:PRO:O	1:B:352:VAL:HG23	2.18	0.42
1:A:324:ILE:HD11	1:A:350:ILE:HG21	2.00	0.42
1:B:280:HIS:O	1:B:283:LYS:HB2	2.19	0.42
1:A:488:ARG:NH2	1:B:372:ASP:OD1	2.34	0.42
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.84	0.42
1:A:502:ARG:HD3	1:A:512:TRP:CG	2.54	0.42
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.79	0.42
1:A:725:ILE:HD13	1:A:725:ILE:HA	1.84	0.42
1:B:643:LEU:HA	1:B:643:LEU:HD13	1.77	0.42
1:B:503:GLU:O	1:B:506:THR:HG22	2.19	0.42
1:A:685:PHE:CZ	1:A:694:LEU:HD11	2.55	0.42
1:A:349:GLN:NE2	1:A:353:ASN:OD1	2.53	0.42
1:B:391:LEU:HD11	1:B:784:GLN:OE1	2.21	0.41
1:A:701:ASP:HB2	1:A:720:ASN:HD22	1.85	0.41
1:A:659:GLY:O	1:A:694:LEU:HA	2.21	0.41
1:B:761:MET:HE2	1:B:761:MET:HB3	1.94	0.41
1:A:258:LYS:HD3	1:A:438:VAL:HG21	2.01	0.41
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:PRO:HA	1:A:693:ILE:HG23	2.02	0.41
1:B:395:LEU:HD12	1:B:788:LYS:HD3	2.02	0.41
1:B:691:HIS:CD2	1:B:691:HIS:N	2.88	0.41
1:A:307:LYS:HA	1:A:345:ILE:HG13	2.02	0.41
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.89	0.41
1:B:264:ALA:O	1:B:410:ALA:HA	2.20	0.41
1:B:270:LYS:N	2:B:801:SO4:O4	2.41	0.41
1:B:274:SER:HB2	1:B:370:ILE:HD13	2.02	0.41
1:A:781:LEU:HA	1:A:784:GLN:HG3	2.03	0.41
1:B:446:LEU:O	1:B:450:GLU:HG2	2.20	0.41
1:B:466:ARG:CG	1:B:466:ARG:NH2	2.79	0.41
1:B:659:GLY:HA3	1:B:691:HIS:HD1	1.86	0.41
1:A:721:VAL:HG21	1:B:496:LEU:HD13	2.03	0.40
1:B:475:ILE:HB	1:B:552:LEU:HD21	2.04	0.40
1:B:540:LEU:HD12	1:B:540:LEU:HA	1.87	0.40
1:A:580:ASP:HB2	1:A:583:GLU:OE1	2.22	0.40
1:A:685:PHE:HB3	1:A:708:GLN:HB3	2.03	0.40
1:B:442:VAL:HG11	1:B:449:LEU:HD22	2.04	0.40
1:A:686:LYS:H	1:A:686:LYS:HG3	1.63	0.40
1:A:724:MET:HE3	1:A:724:MET:HB2	1.66	0.40
1:B:300:ILE:HD12	1:B:300:ILE:H	1.87	0.40
1:B:387:MET:HE1	1:B:405:VAL:HG21	2.04	0.40
1:B:547:LYS:HG3	1:B:570:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

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	504/580 (87%)	494 (98%)	10 (2%)	0	100	100
1	B	481/580 (83%)	473 (98%)	7 (2%)	1 (0%)	43	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	985/1160 (85%)	967 (98%)	17 (2%)	1 (0%)	48 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	PHE

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	461/518 (89%)	401 (87%)	60 (13%)	4 10
1	B	449/518 (87%)	385 (86%)	64 (14%)	3 7
All	All	910/1036 (88%)	786 (86%)	124 (14%)	3 8

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	A	270	LYS
1	A	307	LYS
1	A	324	ILE
1	A	328	THR
1	A	330	GLU
1	A	335	GLU
1	A	339	GLU
1	A	346	LEU
1	A	357	LYS
1	A	364	SER
1	A	365	ILE
1	A	414	VAL
1	A	418	LYS
1	A	420	THR
1	A	433	SER
1	A	442	VAL

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Mol	Chain	Res	Type
1	A	446	LEU
1	A	455	LYS
1	A	461	ARG
1	A	479	MET
1	A	485	LEU
1	A	491	LYS
1	A	498	GLN
1	A	511	GLN
1	A	518	LYS
1	A	533	ARG
1	A	535	CYS
1	A	536	LYS
1	A	540	LEU
1	A	552	LEU
1	A	573	ASN
1	A	579	PHE
1	A	580	ASP
1	A	584	GLN
1	A	588	GLN
1	A	594	LEU
1	A	600	VAL
1	A	605	SER
1	A	614	LEU
1	A	624	LEU
1	A	643	LEU
1	A	661	LEU
1	A	686	LYS
1	A	690	ASP
1	A	704	ILE
1	A	710	ASN
1	A	721	VAL
1	A	724	MET
1	A	725	ILE
1	A	737	LYS
1	A	742	THR
1	A	748	ILE
1	A	759	LYS
1	A	764	SER
1	A	769	GLN
1	A	781	LEU
1	A	784	GLN
1	A	788	LYS

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Mol	Chain	Res	Type
1	A	790	ILE
1	B	249	GLU
1	B	255	MET
1	B	261	ILE
1	B	266	THR
1	B	277	ILE
1	B	316	ARG
1	B	324	ILE
1	B	331	ASN
1	B	332	VAL
1	B	357	LYS
1	B	363	LEU
1	B	378	SER
1	B	387	MET
1	B	391	LEU
1	B	399	SER
1	B	416	ASP
1	B	442	VAL
1	B	446	LEU
1	B	451	GLN
1	B	462	LYS
1	B	466	ARG
1	B	472	LYS
1	B	484	SER
1	B	491	LYS
1	B	494	GLU
1	B	496	LEU
1	B	497	SER
1	B	498	GLN
1	B	500	GLN
1	B	502	ARG
1	B	503	GLU
1	B	507	GLN
1	B	517	GLN
1	B	522	VAL
1	B	523	PHE
1	B	528	LYS
1	B	529	ASP
1	B	532	SER
1	B	546	ARG
1	B	568	LYS
1	B	575	ARG

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Mol	Chain	Res	Type
1	B	579	PHE
1	B	583	GLU
1	B	594	LEU
1	B	599	SER
1	B	627	GLU
1	B	629	ILE
1	B	637	ARG
1	B	643	LEU
1	B	695	ILE
1	B	697	THR
1	B	706	ILE
1	B	711	LEU
1	B	714	LEU
1	B	740	LEU
1	B	741	LEU
1	B	752	GLN
1	B	754	ASN
1	B	759	LYS
1	B	766	LEU
1	B	772	ASP
1	B	780	ILE
1	B	788	LYS
1	B	793	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	708	GLN
1	A	720	ASN
1	B	336	GLN
1	B	354	ASN
1	B	376	ASN
1	B	445	ASN
1	B	498	GLN
1	B	517	GLN
1	B	769	GLN
1	B	784	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	SO4	A	802	-	4,4,4	0.89	0	6,6,6	0.19	0
2	SO4	B	801	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	A	801	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	B	802	-	4,4,4	0.26	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	SO4	1	0
2	A	801	SO4	2	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	514/580 (88%)	0.34	29 (5%)	30 27	25, 59, 91, 148	166 (32%)
1	B	495/580 (85%)	0.54	43 (8%)	16 14	27, 64, 97, 140	198 (40%)
All	All	1009/1160 (86%)	0.44	72 (7%)	22 19	25, 61, 95, 148	364 (36%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	VAL	6.7
1	A	703	GLY	5.0
1	A	578	GLY	5.0
1	B	707	ALA	4.9
1	B	396	GLY	4.6
1	B	776	PHE	4.4
1	B	336	GLN	4.3
1	B	285	PHE	4.2
1	A	332	VAL	4.0
1	B	706	ILE	3.9
1	B	523	PHE	3.8
1	A	329	ALA	3.8
1	B	400	GLY	3.7
1	B	442	VAL	3.7
1	B	512	TRP	3.5
1	B	272	PHE	3.4
1	B	399	SER	3.4
1	B	782	HIS	3.3
1	B	333	PRO	3.3
1	A	579	PHE	3.3
1	A	431	CYS	3.2
1	A	661	LEU	3.1
1	A	331	ASN	3.1
1	A	241	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	788	LYS	2.9
1	B	720	ASN	2.9
1	B	433	SER	2.9
1	A	789	PHE	2.8
1	B	721	VAL	2.8
1	A	497	SER	2.8
1	B	290	LYS	2.8
1	B	282	LEU	2.8
1	B	502	ARG	2.6
1	B	428	CYS	2.6
1	A	353	ASN	2.6
1	B	688	SER	2.5
1	B	579	PHE	2.5
1	A	528	LYS	2.5
1	A	704	ILE	2.5
1	A	771	TRP	2.5
1	B	331	ASN	2.4
1	B	252	LEU	2.4
1	A	522	VAL	2.4
1	B	660	ILE	2.4
1	B	406	ILE	2.4
1	A	324	ILE	2.3
1	A	498	GLN	2.3
1	A	606	ASN	2.3
1	A	689	GLY	2.3
1	B	520	CYS	2.3
1	B	337	ILE	2.3
1	B	499	ILE	2.3
1	A	363	LEU	2.3
1	B	524	GLN	2.2
1	B	367	THR	2.2
1	B	495	ASN	2.2
1	B	334	VAL	2.2
1	A	348	PRO	2.2
1	B	401	PRO	2.2
1	B	267	GLY	2.2
1	B	719	GLY	2.2
1	A	688	SER	2.2
1	B	286	PRO	2.1
1	A	521	MET	2.1
1	B	385	MET	2.1
1	A	325	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	689	GLY	2.1
1	A	328	THR	2.0
1	A	346	LEU	2.0
1	B	509	TYR	2.0
1	B	366	PHE	2.0
1	A	512	TRP	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
3	CL	B	803	1/1	0.59	0.19	145,145,145,145	0
2	SO4	B	802	5/5	0.86	0.09	33,36,40,47	5
2	SO4	A	802	5/5	0.88	0.17	66,71,77,142	0
2	SO4	B	801	5/5	0.92	0.11	69,71,83,88	0
2	SO4	A	801	5/5	0.96	0.09	48,49,54,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.