



# Full wwPDB X-ray Structure Validation Report

Jul 29, 2014 – 01:20 PM EDT

PDB ID : 4ON9  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

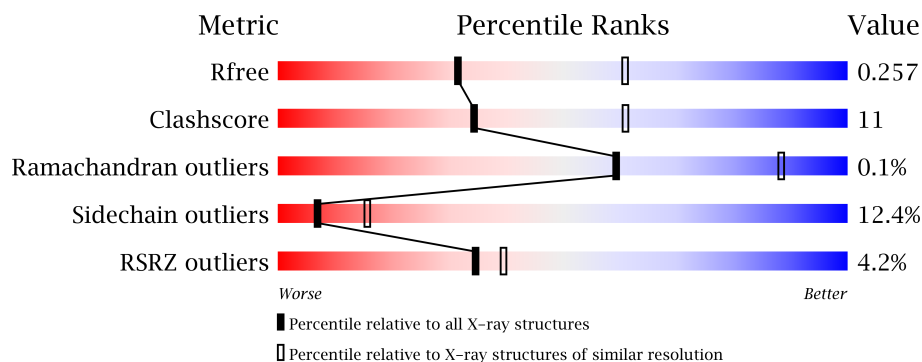
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
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) : stable23489

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1770 (2.74-2.70)
Clashscore	79885	2183 (2.74-2.70)
Ramachandran outliers	78287	2147 (2.74-2.70)
Sidechain outliers	78261	2148 (2.74-2.70)
RSRZ outliers	66119	1772 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	580	
1	B	580	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	B	803	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8183 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 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:

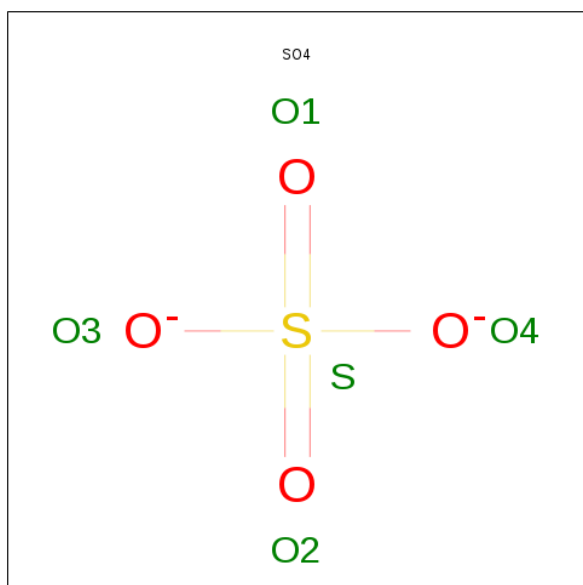
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	EXPRESSION TAG	UNP O95786
A	215	GLY	-	EXPRESSION TAG	UNP O95786
A	216	SER	-	EXPRESSION TAG	UNP O95786
A	217	SER	-	EXPRESSION TAG	UNP O95786
A	218	HIS	-	EXPRESSION TAG	UNP O95786
A	219	HIS	-	EXPRESSION TAG	UNP O95786
A	220	HIS	-	EXPRESSION TAG	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

*Continued on next page...*

Continued from previous page...

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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.1 (49.06-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.219 , 0.258 0.219 , 0.257	Depositor DCC
$R_{free}$ test set	1885 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 57.6	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 38274 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities 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: 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	0.29	0/4203	0.47	0/5662
1	B	0.32	0/4067	0.50	0/5478
All	All	0.31	0/8270	0.49	0/11140

There are no bond length outliers.

There are no bond angle outliers.

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	4130	0	4177	80	0
1	B	3996	0	4038	98	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
4	B	18	0	0	1	0
All	All	8183	0	8215	173	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 11.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:724:MET:HE1	1:A:738:CYS:HB2	1.64	0.79
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:HG3	1:B:466:ARG:HH21	1.52	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:B:454:TYR:HH	1:B:736:SER:H	1.39	0.70
1:A:258:LYS:NZ	1:A:773:GLU:OE2	2.26	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:A:397:GLY:HA2	1:A:398:SER:C	2.17	0.64
1:B:525:MET:HG2	1:B:531:GLU:HB2	1.80	0.64
1:A:477:GLN:OE1	1:A:480:ARG:NH1	2.31	0.63
1:B:466:ARG:CG	1:B:466:ARG:HH21	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:CB	1:A:533:ARG:HH11	2.14	0.60
1:A:500:GLN:HG2	1:B:719:GLY:HA2	1.83	0.59
1:A:442:VAL:HG11	1:A:449:LEU:HD22	1.82	0.59
1:B:284:LYS:HG2	1:B:286:PRO:HD2	1.85	0.58
1:A:335:GLU:CD	1:A:335:GLU:H	2.06	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:377:THR:O	1:B:377:THR:OG1	2.23	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: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:NE2	1:A:349:GLN:O	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: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:271:THR:HG21	1:B:306:GLN:CD	2.33	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:B:778:GLU:CD	1:B:778:GLU:H	2.16	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:335:GLU:HA	1:A:338:VAL:HG12	1.97	0.47
1:A:320:ARG:HD2	1:A:340:ASN:O	2.15	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: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
1:A:596:GLU:O	1:A:600:VAL:HG13	2.17	0.45
1:A:270:LYS:N	2:A:801:SO4:O3	2.48	0.45
1:B:466:ARG:HE	1:B:560:MET:CE	2.29	0.45
1:B:325:SER:C	1:B:350:ILE:HD11	2.37	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: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:B:256:LYS:HB2	1:B:258:LYS:HE2	1.99	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:503:GLU:O	1:B:509:TYR:HB2	2.17	0.44
1:B:579:PHE:HA	1:B:579:PHE:HD1	1.69	0.43
1:A:299:GLN:HB2	1:A:301:PRO:HD2	2.01	0.43
1:A:269:GLY:O	1:A:273:VAL:HG23	2.19	0.43
1:B:306:GLN:OE1	1:B:306:GLN:HA	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:OG	1:A:398:SER:O	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:611:LEU:HD12	1:A:611:LEU:HA	1.84	0.42
1:A:488:ARG:NH2	1:B:372:ASP:OD1	2.34	0.42
1:A:502:ARG:HD3	1:A:512:TRP:CG	2.54	0.42
1:A:446:LEU:HA	1:A:446:LEU:HD12	1.79	0.42
1:A:725:ILE:HD13	1:A:725:ILE:HA	1.84	0.42
1:B:643:LEU:HD13	1:B:643:LEU:HA	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: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
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:B:274:SER:HB2	1:B:370:ILE:HD13	2.02	0.41
1:B:264:ALA:O	1:B:410:ALA:HA	2.20	0.41
1:A:307:LYS:HA	1:A:345:ILE:HG13	2.02	0.41
1:A:493:LEU:HA	1:A:493:LEU:HD12	1.89	0.41
1:B:270:LYS:N	2:B:801:SO4:O4	2.41	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:300:ILE:HD12	1:B:300:ILE:H	1.87	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

### 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	504/580 (87%)	494 (98%)	10 (2%)	0	100	100
1	B	481/580 (83%)	473 (98%)	7 (2%)	1 (0%)	56	85
All	All	985/1160 (85%)	967 (98%)	17 (2%)	1 (0%)	59	88

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%)	407 (88%)	54 (12%)	8	18

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	449/518 (87%)	390 (87%)	59 (13%)	6	14
All	All	910/1036 (88%)	797 (88%)	113 (12%)	7	16

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	PHE
1	A	242	LYS
1	A	244	ARG
1	A	307	LYS
1	A	324	ILE
1	A	328	THR
1	A	335	GLU
1	A	339	GLU
1	A	346	LEU
1	A	364	SER
1	A	365	ILE
1	A	414	VAL
1	A	416	ASP
1	A	418	LYS
1	A	420	THR
1	A	433	SER
1	A	442	VAL
1	A	446	LEU
1	A	455	LYS
1	A	485	LEU
1	A	488	ARG
1	A	491	LYS
1	A	498	GLN
1	A	510	GLU
1	A	511	GLN
1	A	518	LYS
1	A	533	ARG
1	A	535	CYS
1	A	540	LEU
1	A	546	ARG
1	A	552	LEU
1	A	579	PHE
1	A	580	ASP
1	A	584	GLN
1	A	588	GLN
1	A	594	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	605	SER
1	A	643	LEU
1	A	652	LYS
1	A	686	LYS
1	A	690	ASP
1	A	704	ILE
1	A	721	VAL
1	A	737	LYS
1	A	742	THR
1	A	748	ILE
1	A	764	SER
1	A	769	GLN
1	A	781	LEU
1	A	782	HIS
1	A	784	GLN
1	A	788	LYS
1	A	789	PHE
1	A	790	ILE
1	B	244	ARG
1	B	249	GLU
1	B	255	MET
1	B	261	ILE
1	B	266	THR
1	B	277	ILE
1	B	283	LYS
1	B	290	LYS
1	B	316	ARG
1	B	324	ILE
1	B	331	ASN
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	424	LEU
1	B	446	LEU
1	B	451	GLN
1	B	462	LYS
1	B	466	ARG
1	B	472	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	484	SER
1	B	488	ARG
1	B	491	LYS
1	B	494	GLU
1	B	497	SER
1	B	498	GLN
1	B	502	ARG
1	B	507	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
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	695	ILE
1	B	697	THR
1	B	711	LEU
1	B	714	LEU
1	B	740	LEU
1	B	752	GLN
1	B	754	ASN
1	B	755	MET
1	B	766	LEU
1	B	772	ASP
1	B	780	ILE
1	B	793	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	349	GLN
1	A	708	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	720	ASN
1	B	498	GLN
1	B	500	GLN
1	B	517	GLN
1	B	769	GLN

### 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 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	801	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	A	802	-	4,4,4	1.30	0	6,6,6	0.24	0
2	SO4	B	801	-	4,4,4	0.31	0	6,6,6	0.42	0
2	SO4	B	802	-	4,4,4	0.12	0	6,6,6	0.09	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	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0

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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	514/580 (88%)	-0.15	6 (1%) 75 81	36, 64, 106, 172	167 (32%)
1	B	495/580 (85%)	0.17	36 (7%) 15 16	32, 71, 112, 151	204 (41%)
All	All	1009/1160 (86%)	0.00	42 (4%) 35 39	32, 67, 112, 172	371 (36%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	PHE	8.1
1	A	497	SER	7.2
1	B	719	GLY	6.6
1	B	331	ASN	6.4
1	A	498	GLN	5.8
1	B	282	LEU	5.8
1	B	286	PRO	5.0
1	B	291	GLY	4.3
1	B	336	GLN	4.0
1	B	338	VAL	3.7
1	B	334	VAL	3.7
1	B	406	ILE	3.5
1	B	333	PRO	3.4
1	A	499	ILE	3.4
1	B	721	VAL	3.4
1	B	452	VAL	3.4
1	A	329	ALA	3.3
1	B	442	VAL	3.2
1	B	337	ILE	3.1
1	B	260	THR	3.0
1	A	687	ALA	2.9
1	B	789	PHE	2.9
1	B	695	ILE	2.8
1	B	243	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	332	VAL	2.8
1	B	363	LEU	2.7
1	B	313	TYR	2.6
1	B	283	LYS	2.6
1	B	312	LYS	2.5
1	B	428	CYS	2.4
1	B	520	CYS	2.4
1	B	401	PRO	2.4
1	B	319	TYR	2.4
1	B	248	LEU	2.4
1	A	578	GLY	2.3
1	B	290	LYS	2.3
1	B	272	PHE	2.2
1	B	244	ARG	2.2
1	B	454	TYR	2.1
1	B	502	ARG	2.0
1	B	788	LYS	2.0
1	B	427	ILE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CL	B	803	1/1	0.42	19.76	145,145,145,145	0
2	SO4	A	801	5/5	0.20	1.35	48,49,54,57	0
2	SO4	B	802	5/5	0.24	0.49	33,36,40,47	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	801	5/5	0.14	-1.10	69,71,83,88	0
2	SO4	A	802	5/5	0.13	-1.56	66,71,77,142	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.