



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:45 AM GMT

PDB ID : 3KSK
Title : Crystal Structure of single chain PvuII
Authors : Meramveliotaki, C.; Hountas, A.; Eliopoulos, E.; Kokkinidis, M.
Deposited on : 2009-11-23
Resolution : 2.35 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>

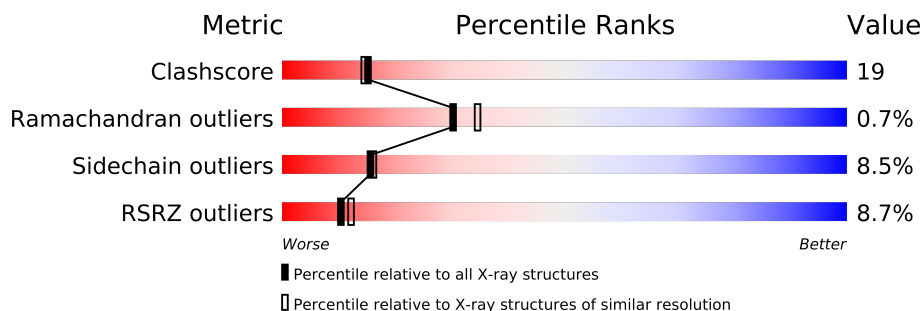
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	324	
1	B	324	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	326	-	X
2	SO4	B	327	-	X
3	MPD	A	328	-	X
4	TRS	B	329	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5633 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 Type-2 restriction enzyme PvuII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2572	1670	435	463	4			
1	B	311	Total	C	N	O	S	0	0	0
			2543	1651	428	460	4			

There are 24 discrepancies between the modelled and reference sequences:

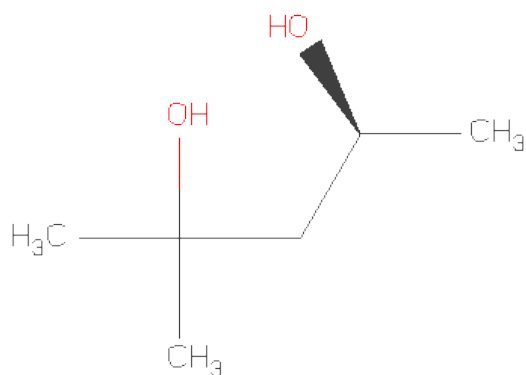
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	LINKER	UNP P23657
A	159	SER	-	LINKER	UNP P23657
A	160	GLY	-	LINKER	UNP P23657
A	161	GLY	-	LINKER	UNP P23657
A	318	GLY	-	EXPRESSION TAG	UNP P23657
A	319	SER	-	EXPRESSION TAG	UNP P23657
A	320	HIS	-	EXPRESSION TAG	UNP P23657
A	321	HIS	-	EXPRESSION TAG	UNP P23657
A	322	HIS	-	EXPRESSION TAG	UNP P23657
A	323	HIS	-	EXPRESSION TAG	UNP P23657
A	324	HIS	-	EXPRESSION TAG	UNP P23657
A	325	HIS	-	EXPRESSION TAG	UNP P23657
B	158	GLY	-	LINKER	UNP P23657
B	159	SER	-	LINKER	UNP P23657
B	160	GLY	-	LINKER	UNP P23657
B	161	GLY	-	LINKER	UNP P23657
B	318	GLY	-	EXPRESSION TAG	UNP P23657
B	319	SER	-	EXPRESSION TAG	UNP P23657
B	320	HIS	-	EXPRESSION TAG	UNP P23657
B	321	HIS	-	EXPRESSION TAG	UNP P23657
B	322	HIS	-	EXPRESSION TAG	UNP P23657
B	323	HIS	-	EXPRESSION TAG	UNP P23657
B	324	HIS	-	EXPRESSION TAG	UNP P23657
B	325	HIS	-	EXPRESSION TAG	UNP P23657

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



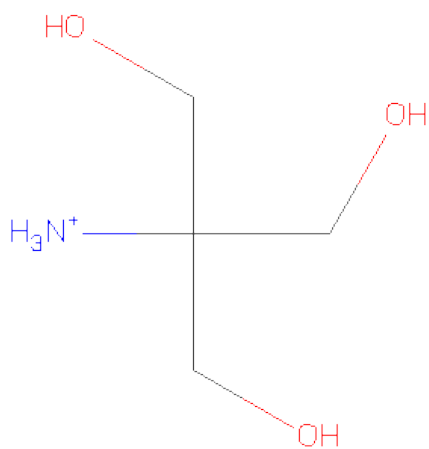
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 5 is water.

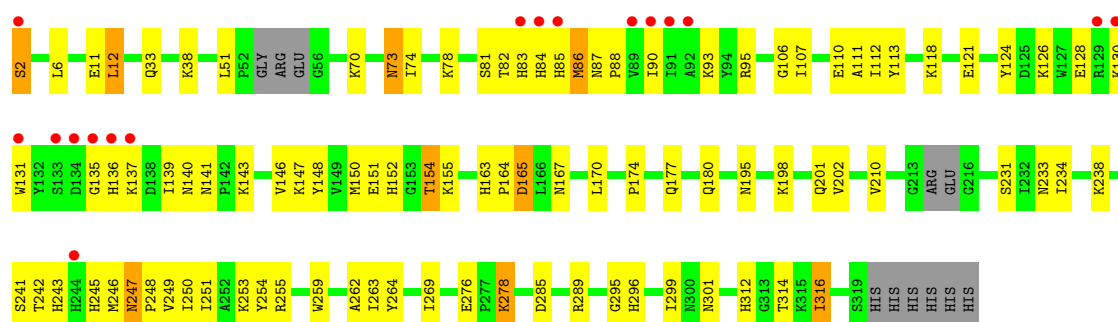
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	274	Total 274	O 274	0	0
5	B	195	Total 195	O 195	0	0

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.

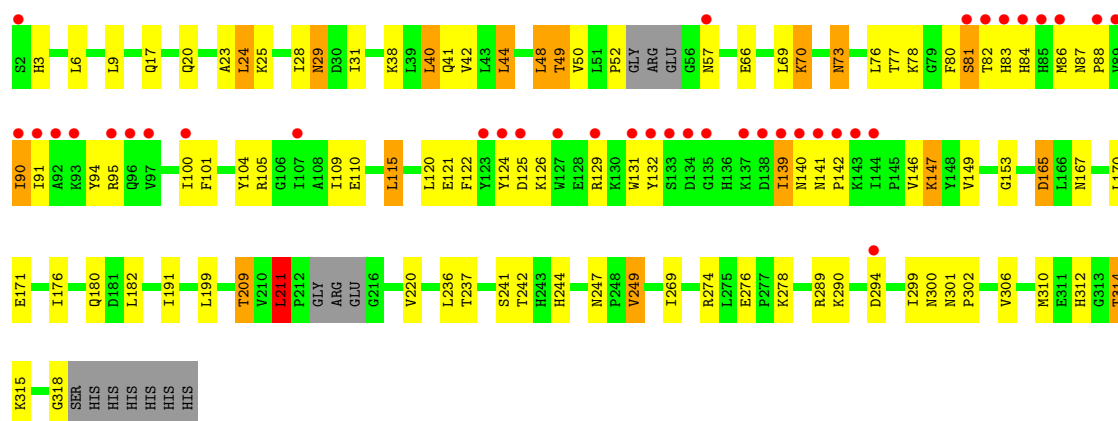
• Molecule 1: Type-2 restriction enzyme PvuII

Chain A: 



• Molecule 1: Type-2 restriction enzyme PvuII

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	101.92Å 101.92Å 100.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.06 – 2.35 31.76 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.6 (102.06-2.35) 98.6 (31.76-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.283 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
Estimated twinning fraction	0.011 for -h,-l,-k 0.000 for -h,l,k 0.000 for l,-k,h 0.003 for -l,-k,-h 0.023 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 42168 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5633	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MPD, TRS, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/2650	0.97	4/3595 (0.1%)
1	B	0.53	0/2616	1.02	5/3553 (0.1%)
All	All	0.53	0/5266	1.00	9/7148 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	LEU	CA-CB-CG	14.31	148.21	115.30
1	B	165	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	165	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	316	ILE	CG1-CB-CG2	-6.68	96.69	111.40
1	B	120	LEU	CA-CB-CG	6.17	129.49	115.30
1	B	211	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	69	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	12	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	143	LYS	CD-CE-NZ	-5.09	99.99	111.70

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	2572	0	2529	102	0
1	B	2543	0	2484	92	0
2	A	10	0	0	1	0
2	B	15	0	0	0	0
3	A	8	0	14	15	0
4	B	16	0	24	1	0
5	A	274	0	0	14	0
5	B	195	0	0	14	0
All	All	5633	0	5051	193	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 19.

All (193) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155:LYS:HE3	3:A:328:MPD:C5	1.69	1.20
1:A:155:LYS:HE3	3:A:328:MPD:H53	1.29	1.09
1:A:155:LYS:CE	3:A:328:MPD:H53	1.87	1.05
1:B:29:ASN:ND2	5:B:519:HOH:O	1.93	1.01
1:B:3:HIS:CD2	5:B:379:HOH:O	2.13	1.01
1:B:29:ASN:H	1:B:29:ASN:ND2	1.54	0.99
1:A:238:LYS:HE3	1:B:49:THR:HG21	1.46	0.98
1:B:49:THR:HG22	5:B:404:HOH:O	1.64	0.96
1:A:155:LYS:HE3	3:A:328:MPD:H51	1.47	0.92
1:A:81:SER:HB2	1:A:141:ASN:HD21	1.33	0.92
1:A:111:ALA:HA	3:A:328:MPD:C5	2.01	0.90
1:B:241:SER:HB2	1:B:301:ASN:HD21	1.36	0.90
1:B:274:ARG:HD3	1:B:276:GLU:OE2	1.73	0.89
1:B:29:ASN:HD22	1:B:29:ASN:N	1.68	0.88
1:A:247:ASN:HD22	1:A:249:VAL:H	1.21	0.88
1:B:70:LYS:HD3	1:B:81:SER:O	1.74	0.86
1:B:91:ILE:HG22	1:B:95:ARG:HD2	1.60	0.84
1:A:198:LYS:HZ2	1:A:233:ASN:HD21	1.27	0.82
1:B:29:ASN:HD22	1:B:29:ASN:H	0.87	0.82
1:B:90:ILE:HG13	5:B:496:HOH:O	1.80	0.80
1:B:180:GLN:HE21	1:B:191:ILE:HG12	1.48	0.78
1:A:111:ALA:HA	3:A:328:MPD:C4	2.13	0.78
1:B:147:LYS:N	1:B:147:LYS:HD3	1.98	0.78
1:B:147:LYS:H	1:B:147:LYS:HD3	1.48	0.76
1:A:198:LYS:NZ	1:A:233:ASN:HD21	1.84	0.76
1:B:242:THR:H	1:B:301:ASN:ND2	1.85	0.75
1:A:246:MET:CE	1:A:251:ILE:HG13	2.16	0.75
1:B:236:LEU:HD12	5:B:459:HOH:O	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:ALA:HA	3:A:328:MPD:H51	1.67	0.75
1:A:33:GLN:HG2	5:A:476:HOH:O	1.87	0.74
1:B:115:LEU:HD22	1:B:153:GLY:HA2	1.69	0.74
1:B:3:HIS:HD2	5:B:379:HOH:O	1.56	0.73
1:A:2:SER:N	5:A:350:HOH:O	2.21	0.73
1:B:242:THR:H	1:B:301:ASN:HD21	1.36	0.73
1:A:233:ASN:HB3	5:A:329:HOH:O	1.87	0.73
1:B:29:ASN:N	1:B:29:ASN:ND2	2.32	0.72
1:B:115:LEU:HD22	1:B:153:GLY:CA	2.19	0.71
1:A:111:ALA:HA	3:A:328:MPD:H4	1.73	0.70
1:A:163:HIS:HD2	1:A:165:ASP:H	1.40	0.69
1:A:74:ILE:O	1:A:78:LYS:NZ	2.25	0.69
1:A:276:GLU:CB	1:A:278:LYS:HE2	2.23	0.69
1:A:247:ASN:ND2	1:A:249:VAL:H	1.90	0.69
1:A:174:PRO:HA	1:A:177:GLN:HE21	1.58	0.67
1:B:314:THR:CG2	5:B:440:HOH:O	2.41	0.67
1:B:86:MET:HG2	5:B:518:HOH:O	1.93	0.67
1:B:131:TRP:HD1	1:B:132:TYR:CD1	2.13	0.66
1:B:57:ASN:HB3	1:B:66:GLU:HG2	1.75	0.66
1:B:91:ILE:O	1:B:95:ARG:HG3	1.94	0.66
1:B:315:LYS:HE2	1:B:318:GLY:HA3	1.77	0.66
1:A:33:GLN:CG	5:A:476:HOH:O	2.42	0.65
1:B:180:GLN:NE2	1:B:191:ILE:HG12	2.11	0.65
1:B:241:SER:HB2	1:B:301:ASN:ND2	2.10	0.65
1:A:81:SER:HB2	1:A:141:ASN:ND2	2.09	0.65
1:A:285:ASP:OD2	1:A:289:ARG:NH1	2.30	0.64
1:B:180:GLN:HE22	1:B:191:ILE:H	1.44	0.64
1:A:246:MET:HE1	1:A:251:ILE:HG13	1.78	0.64
1:A:312:HIS:HE1	5:A:349:HOH:O	1.80	0.63
1:A:195:ASN:OD1	1:A:198:LYS:HE3	1.98	0.63
1:A:155:LYS:HE2	3:A:328:MPD:H53	1.79	0.63
1:A:246:MET:HE2	1:A:251:ILE:HG13	1.80	0.63
1:A:124:TYR:O	1:A:128:GLU:HG2	1.98	0.62
1:A:111:ALA:CB	3:A:328:MPD:H51	2.30	0.62
1:A:86:MET:CE	1:A:90:ILE:CG2	2.78	0.62
1:B:126:LYS:NZ	1:B:126:LYS:HB3	2.12	0.62
1:B:57:ASN:CB	1:B:66:GLU:HG2	2.29	0.62
1:A:111:ALA:CA	3:A:328:MPD:H51	2.31	0.61
1:B:314:THR:HG23	5:B:440:HOH:O	2.00	0.61
1:A:95:ARG:HG2	1:A:124:TYR:CD2	2.36	0.60
1:B:147:LYS:H	1:B:147:LYS:CD	2.15	0.60
1:A:131:TRP:CD1	1:A:137:LYS:O	2.54	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:HIS:CD2	1:A:165:ASP:H	2.20	0.60
1:A:242:THR:H	1:A:301:ASN:ND2	2.00	0.60
1:A:154:THR:HG23	5:A:602:HOH:O	2.00	0.59
1:A:155:LYS:CE	3:A:328:MPD:C5	2.54	0.58
1:A:82:THR:H	1:A:141:ASN:ND2	2.01	0.58
1:B:91:ILE:O	1:B:95:ARG:CG	2.51	0.58
1:A:238:LYS:CE	1:B:49:THR:HG21	2.30	0.57
1:A:246:MET:HE3	1:A:250:ILE:HB	1.87	0.57
1:B:48:LEU:HD21	1:B:100:ILE:CD1	2.34	0.57
1:A:233:ASN:ND2	5:A:329:HOH:O	2.36	0.57
1:A:276:GLU:HB2	1:A:278:LYS:HE2	1.86	0.57
1:A:82:THR:HG22	1:A:83:HIS:N	2.19	0.56
1:A:147:LYS:HE2	1:A:147:LYS:H	1.70	0.56
1:A:85:HIS:HD2	5:A:356:HOH:O	1.87	0.56
1:A:247:ASN:HD22	1:A:249:VAL:N	1.96	0.56
1:B:139:ILE:O	5:B:518:HOH:O	2.17	0.56
1:A:247:ASN:HB2	1:A:248:PRO:HD2	1.87	0.56
1:A:139:ILE:HD12	1:A:139:ILE:H	1.71	0.56
1:A:245:HIS:O	1:A:250:ILE:CD1	2.54	0.56
1:A:110:GLU:O	3:A:328:MPD:H52	2.07	0.55
1:A:276:GLU:HB3	1:A:278:LYS:HE2	1.87	0.55
1:A:86:MET:CE	1:A:90:ILE:HG22	2.36	0.55
1:B:299:ILE:HG22	1:B:302:PRO:HD3	1.89	0.55
1:A:86:MET:HE3	1:A:90:ILE:HG21	1.89	0.54
1:B:84:HIS:HA	1:B:141:ASN:H	1.73	0.54
1:A:202:VAL:HG22	1:A:269:ILE:HD13	1.88	0.54
1:B:139:ILE:H	1:B:139:ILE:HD12	1.72	0.54
1:A:198:LYS:NZ	1:A:233:ASN:ND2	2.55	0.54
1:A:70:LYS:HD2	1:A:81:SER:O	2.08	0.54
1:B:141:ASN:HB3	5:B:360:HOH:O	2.07	0.53
1:A:87:ASN:HB2	1:A:88:PRO:CD	2.38	0.53
1:B:167:ASN:O	1:B:171:GLU:HG3	2.08	0.53
1:B:247:ASN:OD1	1:B:249:VAL:HG13	2.09	0.53
1:B:209:THR:HG22	1:B:220:VAL:HG13	1.91	0.53
1:B:78:LYS:O	1:B:146:VAL:HG23	2.09	0.53
1:B:87:ASN:HB2	1:B:88:PRO:CD	2.39	0.53
1:B:20:GLN:HE21	1:B:31:ILE:HG12	1.75	0.52
1:B:211:LEU:HD13	1:B:220:VAL:HG12	1.90	0.52
1:A:38:LYS:HE2	1:A:107:ILE:HA	1.92	0.51
1:B:180:GLN:NE2	1:B:191:ILE:H	2.08	0.51
1:A:251:ILE:HG22	1:A:255:ARG:HH22	1.76	0.51
1:A:90:ILE:O	1:A:93:LYS:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LYS:H	1:A:278:LYS:NZ	2.09	0.50
1:B:80:PHE:HE1	1:B:146:VAL:HG13	1.77	0.50
1:B:312:HIS:HE1	5:B:332:HOH:O	1.94	0.49
1:B:82:THR:OG1	1:B:142:PRO:HD2	2.12	0.49
1:B:129:ARG:HA	1:B:129:ARG:NE	2.28	0.49
1:B:73:ASN:HD22	1:B:73:ASN:C	2.14	0.49
1:A:246:MET:HB3	1:A:299:ILE:HB	1.93	0.49
1:B:131:TRP:HH2	5:B:373:HOH:O	1.95	0.49
1:B:306:VAL:O	1:B:310:MET:HG3	2.12	0.49
1:A:164:PRO:O	1:A:167:ASN:ND2	2.46	0.49
1:A:95:ARG:HH22	1:A:128:GLU:CD	2.16	0.49
1:B:80:PHE:CD2	1:B:101:PHE:HD2	2.31	0.49
1:A:137:LYS:HD3	1:A:137:LYS:O	2.13	0.48
1:A:295:GLY:O	1:A:296:HIS:HB2	2.12	0.48
1:B:25:LYS:HE3	1:B:165:ASP:OD2	2.13	0.48
1:B:91:ILE:O	1:B:95:ARG:CD	2.61	0.48
1:A:86:MET:CE	1:A:90:ILE:HG21	2.41	0.48
1:A:233:ASN:OD1	5:A:482:HOH:O	2.20	0.48
1:B:122:PHE:CZ	1:B:126:LYS:HD2	2.49	0.48
1:A:198:LYS:HZ2	1:A:233:ASN:ND2	2.04	0.48
1:A:139:ILE:HD12	1:A:139:ILE:N	2.28	0.48
2:A:326:SO4:O2	5:A:556:HOH:O	2.20	0.48
1:A:278:LYS:H	1:A:278:LYS:HZ3	1.61	0.47
1:A:201:GLN:NE2	1:A:269:ILE:HG22	2.30	0.47
1:B:170:LEU:HD23	4:B:329:TRS:H31	1.96	0.47
1:B:147:LYS:N	1:B:147:LYS:CD	2.73	0.47
1:A:73:ASN:HD21	1:A:106:GLY:H	1.63	0.47
1:A:251:ILE:HG22	1:A:255:ARG:NH2	2.30	0.47
1:A:234:ILE:HB	1:A:263:ILE:HG23	1.98	0.46
1:B:91:ILE:HA	1:B:94:TYR:HB2	1.96	0.46
1:B:91:ILE:HG21	1:B:124:TYR:HB3	1.97	0.46
1:A:146:VAL:O	1:A:150:MET:HG3	2.15	0.46
1:A:241:SER:HB3	1:A:301:ASN:HD21	1.81	0.46
1:A:86:MET:HE3	1:A:90:ILE:CG2	2.46	0.46
1:B:244:HIS:O	1:B:300:ASN:HA	2.16	0.46
1:B:83:HIS:HB3	1:B:86:MET:HB3	1.98	0.46
1:B:91:ILE:HG22	1:B:95:ARG:HH11	1.81	0.45
1:A:247:ASN:HB2	1:A:248:PRO:CD	2.46	0.45
1:B:125:ASP:O	1:B:129:ARG:HG2	2.17	0.45
1:B:126:LYS:HZ3	1:B:126:LYS:HB3	1.80	0.45
1:B:80:PHE:O	1:B:81:SER:C	2.55	0.45
1:A:246:MET:CE	1:A:251:ILE:CG1	2.92	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:48:LEU:HD21	1:B:100:ILE:HD12	1.98	0.45
1:B:3:HIS:CE1	1:B:6:LEU:HB2	2.51	0.45
1:B:90:ILE:HG22	1:B:91:ILE:N	2.32	0.45
1:A:113:TYR:CE1	1:A:155:LYS:HB2	2.52	0.44
3:A:328:MPD:H4	3:A:328:MPD:H12	1.66	0.44
1:A:246:MET:HE1	1:A:251:ILE:CG1	2.46	0.44
1:B:88:PRO:HG2	5:B:480:HOH:O	2.17	0.44
1:A:231:SER:HA	1:A:262:ALA:O	2.18	0.43
1:B:41:GLN:HE21	1:B:109:ILE:HG22	1.83	0.43
1:B:121:GLU:OE2	1:B:121:GLU:HA	2.18	0.43
1:B:274:ARG:CD	1:B:276:GLU:OE2	2.56	0.43
1:B:91:ILE:CG2	1:B:124:TYR:HB3	2.48	0.43
1:A:316:ILE:HD13	1:A:316:ILE:HG21	1.51	0.43
1:A:254:TYR:CD1	1:A:259:TRP:HZ2	2.36	0.43
1:A:86:MET:HE1	1:A:90:ILE:HG22	2.01	0.43
1:B:129:ARG:HA	1:B:129:ARG:HE	1.84	0.42
1:A:82:THR:H	1:A:141:ASN:HD21	1.67	0.42
1:B:38:LYS:HB3	1:B:104:TYR:CE2	2.55	0.42
1:B:95:ARG:HG2	1:B:124:TYR:CD1	2.53	0.42
1:B:76:LEU:HD12	1:B:77:THR:HG22	2.02	0.42
1:B:40:LEU:HD22	1:B:44:LEU:HD22	2.01	0.42
1:B:86:MET:CE	1:B:142:PRO:HG2	2.49	0.42
1:A:152:HIS:HE1	5:A:369:HOH:O	2.03	0.42
1:A:264:TYR:HD2	5:A:482:HOH:O	2.02	0.41
5:A:366:HOH:O	1:B:52:PRO:HG2	2.20	0.41
1:A:242:THR:OG1	1:A:243:HIS:N	2.52	0.41
1:B:23:ALA:HB1	1:B:28:ILE:HB	2.01	0.41
1:B:84:HIS:O	1:B:140:ASN:HA	2.20	0.41
1:A:148:TYR:HA	1:A:151:GLU:HG2	2.02	0.41
1:B:105:ARG:HD2	1:B:110:GLU:OE2	2.21	0.41
1:A:112:ILE:HG13	3:A:328:MPD:H12	2.01	0.41
1:A:238:LYS:HE3	1:B:49:THR:CG2	2.35	0.41
1:A:247:ASN:C	1:A:247:ASN:HD22	2.24	0.41
1:A:95:ARG:NH1	1:A:121:GLU:OE2	2.53	0.41
1:A:242:THR:H	1:A:301:ASN:HD21	1.67	0.41
1:A:314:THR:HG23	5:A:578:HOH:O	2.21	0.41
1:B:211:LEU:HD13	1:B:220:VAL:CG1	2.51	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	308/324 (95%)	298 (97%)	8 (3%)	2 (1%)	33	39
1	B	305/324 (94%)	284 (93%)	19 (6%)	2 (1%)	30	34
All	All	613/648 (95%)	582 (95%)	27 (4%)	4 (1%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	GLY
1	B	81	SER
1	A	136	HIS
1	B	294	ASP

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	275/284 (97%)	258 (94%)	17 (6%)	26	29
1	B	270/284 (95%)	241 (89%)	29 (11%)	10	9
All	All	545/568 (96%)	499 (92%)	46 (8%)	15	17

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	6	LEU
1	A	11	GLU
1	A	12	LEU
1	A	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	ASN
1	A	86	MET
1	A	118	LYS
1	A	126	LYS
1	A	130	LYS
1	A	154	THR
1	A	170	LEU
1	A	180	GLN
1	A	210	VAL
1	A	247	ASN
1	A	253	LYS
1	A	278	LYS
1	B	9	LEU
1	B	17	GLN
1	B	24	LEU
1	B	29	ASN
1	B	40	LEU
1	B	42	VAL
1	B	44	LEU
1	B	48	LEU
1	B	49	THR
1	B	50	VAL
1	B	70	LYS
1	B	73	ASN
1	B	90	ILE
1	B	115	LEU
1	B	139	ILE
1	B	147	LYS
1	B	149	VAL
1	B	176	ILE
1	B	182	LEU
1	B	199	LEU
1	B	209	THR
1	B	211	LEU
1	B	237	THR
1	B	249	VAL
1	B	269	ILE
1	B	278	LYS
1	B	289	ARG
1	B	290	LYS
1	B	314	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	73	ASN
1	A	85	HIS
1	A	163	HIS
1	A	167	ASN
1	A	177	GLN
1	A	180	GLN
1	A	201	GLN
1	A	217	ASN
1	A	222	ASN
1	A	233	ASN
1	A	247	ASN
1	A	256	GLN
1	A	296	HIS
1	A	300	ASN
1	A	301	ASN
1	B	7	ASN
1	B	20	GLN
1	B	29	ASN
1	B	41	GLN
1	B	57	ASN
1	B	62	ASN
1	B	73	ASN
1	B	152	HIS
1	B	180	GLN
1	B	217	ASN
1	B	244	HIS
1	B	301	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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	326	-	4,4,4	0.09	0	6,6,6	0.38	0
2	SO4	A	327	-	4,4,4	0.26	0	6,6,6	0.48	0
3	MPD	A	328	-	7,7,7	0.32	0	10,10,10	1.10	1 (10%)
2	SO4	B	1	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	B	326	-	4,4,4	0.09	0	6,6,6	0.20	0
2	SO4	B	327	-	4,4,4	0.20	0	6,6,6	0.44	0
4	TRS	B	328	-	7,7,7	1.22	1 (14%)	9,9,9	1.81	3 (33%)
4	TRS	B	329	-	7,7,7	0.96	1 (14%)	9,9,9	1.59	2 (22%)

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	326	-	-	0/0/0/0	0/0/0/0
2	SO4	A	327	-	-	0/0/0/0	0/0/0/0
3	MPD	A	328	-	-	0/5/5/5	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	326	-	-	0/0/0/0	0/0/0/0
2	SO4	B	327	-	-	0/0/0/0	0/0/0/0
4	TRS	B	328	-	-	0/9/9/9	0/0/0/0
4	TRS	B	329	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	328	TRS	C-N	-3.09	1.46	1.50
4	B	329	TRS	C-N	-2.45	1.47	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	328	TRS	C3-C-C1	3.42	116.31	110.70
4	B	329	TRS	C3-C-C1	-3.04	105.72	110.70
4	B	328	TRS	C2-C-C1	-2.70	106.27	110.70
4	B	329	TRS	O2-C2-C	-2.64	105.76	111.55
4	B	328	TRS	O2-C2-C	-2.62	105.80	111.55
3	A	328	MPD	O2-C2-CM	2.05	115.73	107.98

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	313/324 (96%)	0.17	17 (5%) 25 28	28, 42, 67, 82	0
1	B	311/324 (95%)	0.58	38 (12%) 5 5	29, 45, 78, 92	0
All	All	624/648 (96%)	0.37	55 (8%) 10 12	28, 43, 74, 92	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	ASP	8.1
1	B	133	SER	7.2
1	B	131	TRP	6.9
1	B	93	LYS	6.5
1	B	139	ILE	6.1
1	B	127	TRP	5.9
1	B	85	HIS	5.4
1	B	86	MET	5.3
1	B	141	ASN	5.2
1	B	143	LYS	4.4
1	B	140	ASN	4.4
1	A	89	VAL	4.1
1	B	88	PRO	3.9
1	A	90	ILE	3.7
1	A	2	SER	3.7
1	A	131	TRP	3.5
1	B	82	THR	3.5
1	B	83	HIS	3.5
1	B	90	ILE	3.4
1	B	89	VAL	3.4
1	A	135	GLY	3.4
1	B	84	HIS	3.4
1	B	138	ASP	3.2
1	A	133	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	83	HIS	3.0
1	B	294	ASP	3.0
1	B	95	ARG	3.0
1	B	142	PRO	2.9
1	B	129	ARG	2.9
1	A	137	LYS	2.7
1	A	136	HIS	2.7
1	B	137	LYS	2.6
1	B	97	VAL	2.6
1	B	135	GLY	2.5
1	B	96	GLN	2.5
1	B	132	TYR	2.5
1	B	92	ALA	2.4
1	B	123	TYR	2.3
1	B	125	ASP	2.3
1	A	244	HIS	2.3
1	A	130	LYS	2.3
1	A	84[A]	HIS	2.3
1	A	134	ASP	2.3
1	A	129	ARG	2.2
1	B	57	ASN	2.2
1	A	92	ALA	2.2
1	A	85	HIS	2.1
1	A	91	ILE	2.1
1	B	91	ILE	2.1
1	B	107	ILE	2.1
1	B	81	SER	2.1
1	B	100	ILE	2.1
1	B	124	TYR	2.1
1	B	2	SER	2.1
1	B	144	ILE	2.1

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
3	MPD	A	328	8/8	0.32	4.66	49,56,57,60	0
2	SO4	B	326	5/5	0.20	4.65	73,73,75,76	0
4	TRS	B	329	8/8	0.30	2.85	62,63,64,64	0
2	SO4	B	327	5/5	0.19	2.16	66,66,69,71	0
4	TRS	B	328	8/8	0.22	1.57	53,53,55,56	0
2	SO4	B	1	5/5	0.13	-0.21	89,90,90,92	0
2	SO4	A	327	5/5	0.09	-1.04	60,63,66,66	0
2	SO4	A	326	5/5	0.10	-1.10	82,82,83,85	0

6.5 Other polymers

There are no such residues in this entry.