



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:08 am BST

PDB ID : 3EZF  
Title : Partition Protein  
Authors : Schumacher, M.A.  
Deposited on : 2008-10-22  
Resolution : 2.80 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

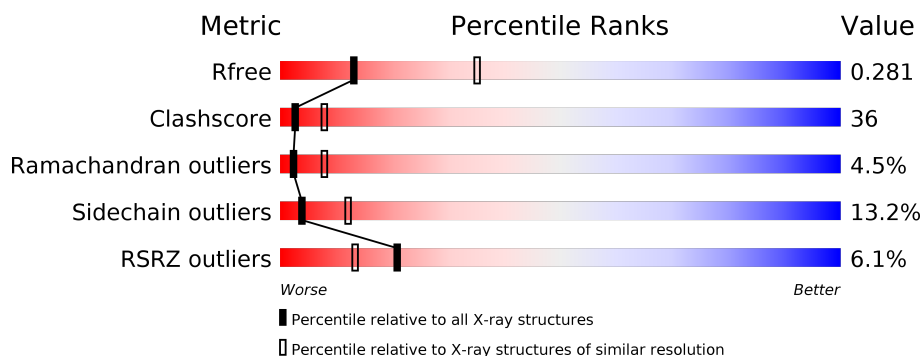
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	403	<div> <div>5%</div> <div>36%</div> <div>41%</div> <div>7%</div> <div>15%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2799 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 ParA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2722	1727	476	512	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP B4ABW6
A	0	MET	-	EXPRESSION TAG	UNP B4ABW6
A	21	ALA	SER	CONFLICT	UNP B4ABW6
A	28	ASP	GLU	CONFLICT	UNP B4ABW6
A	35	GLN	LEU	CONFLICT	UNP B4ABW6
A	59	ASP	GLU	CONFLICT	UNP B4ABW6
A	67	GLU	ASP	CONFLICT	UNP B4ABW6
A	68	ASP	GLY	CONFLICT	UNP B4ABW6
A	71	GLN	GLU	CONFLICT	UNP B4ABW6
A	182	ASN	ASP	CONFLICT	UNP B4ABW6
A	198	VAL	ILE	CONFLICT	UNP B4ABW6
A	218	ARG	GLU	CONFLICT	UNP B4ABW6
A	219	GLU	ASP	CONFLICT	UNP B4ABW6
A	222	GLU	LYS	CONFLICT	UNP B4ABW6
A	228	GLN	MET	CONFLICT	UNP B4ABW6
A	229	ASN	LYS	CONFLICT	UNP B4ABW6
A	230	GLN	PRO	CONFLICT	UNP B4ABW6
A	231	TYR	SER	CONFLICT	UNP B4ABW6
A	233	ILE	VAL	CONFLICT	UNP B4ABW6
A	236	ARG	LYS	CONFLICT	UNP B4ABW6
A	237	ASN	LYS	CONFLICT	UNP B4ABW6
A	240	ASP	GLU	CONFLICT	UNP B4ABW6
A	360	VAL	ILE	CONFLICT	UNP B4ABW6
A	380	THR	ASN	CONFLICT	UNP B4ABW6

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

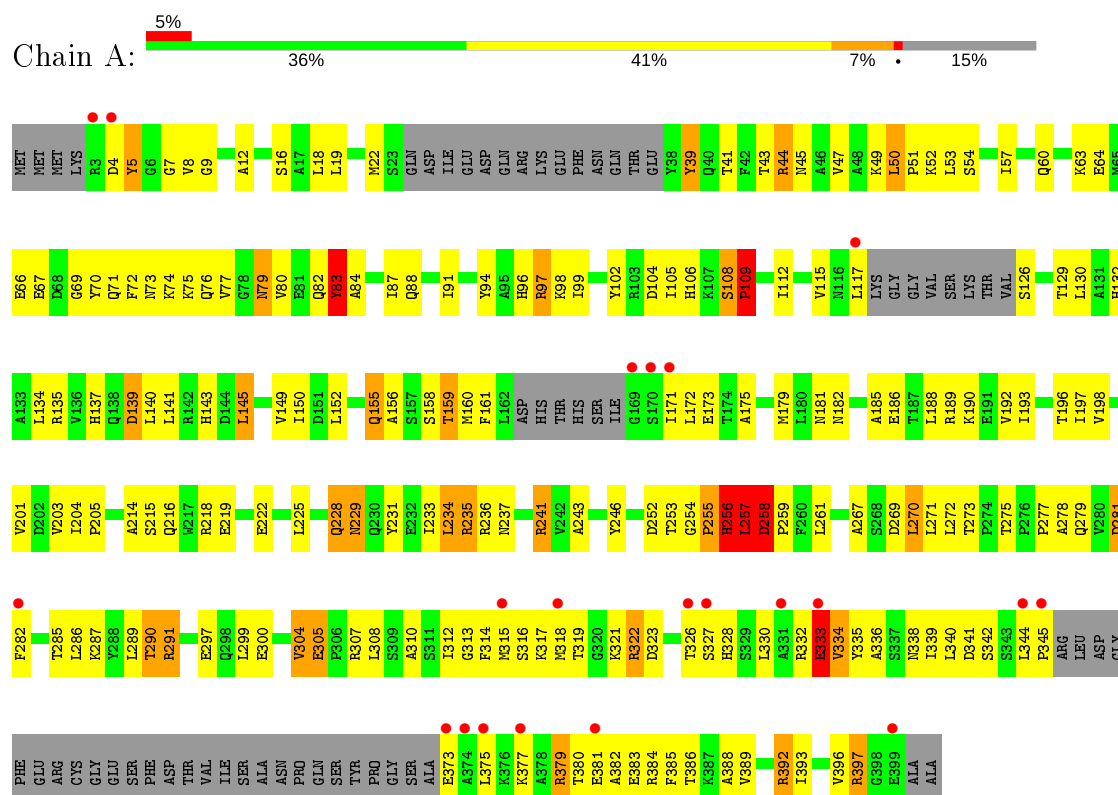
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		

### 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 the various outlier classes 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: ParA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 <sub>2</sub> 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.46 Å   109.46 Å   128.39 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	94.80 – 2.80 94.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (94.80-2.80) 98.4 (94.80-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.82 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.253   ,   0.277 0.257   ,   0.281	Depositor DCC
$R_{free}$ test set	925 reflections (8.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 68.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	3/2770 (0.1%)	0.88	7/3749 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	CG-CD	8.81	1.65	1.51
1	A	219	GLU	CB-CG	7.29	1.66	1.52
1	A	219	GLU	CD-OE1	5.46	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	PRO	CA-N-CD	-27.87	72.48	111.50
1	A	44	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	219	GLU	CG-CD-OE1	7.07	132.43	118.30
1	A	80	VAL	N-CA-CB	-6.31	97.63	111.50
1	A	109	PRO	CA-CB-CG	-5.81	92.95	104.00
1	A	79	ASN	C-N-CA	5.75	136.09	121.70
1	A	44	ARG	NE-CZ-NH2	5.11	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	2722	0	2732	198	1
2	A	35	0	0	2	0
3	A	42	0	0	5	0
All	All	2799	0	2732	198	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 36.

All (198) 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:A:171:ILE:HG22	1:A:172:LEU:N	1.81	0.94
1:A:171:ILE:HG22	1:A:172:LEU:H	1.31	0.94
1:A:173:GLU:HG2	1:A:192:VAL:HG22	1.51	0.91
1:A:137:HIS:HB3	1:A:140:LEU:HB2	1.55	0.88
1:A:229:ASN:HD22	1:A:231:TYR:H	1.20	0.88
1:A:229:ASN:ND2	1:A:231:TYR:H	1.74	0.85
1:A:18:LEU:O	1:A:22:MET:HG2	1.78	0.84
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.42	0.83
1:A:373:GLU:HA	1:A:377:LYS:HD2	1.58	0.83
1:A:171:ILE:CG2	1:A:172:LEU:H	1.93	0.81
1:A:51:PRO:HG2	1:A:139:ASP:HB3	1.60	0.81
1:A:196:THR:HG23	1:A:198:VAL:H	1.45	0.81
1:A:188:LEU:O	1:A:193:ILE:HG12	1.81	0.81
1:A:334:VAL:HG23	1:A:335:TYR:H	1.46	0.80
1:A:43:THR:HG21	2:A:696:SO4:O1	1.80	0.80
1:A:344:LEU:HD12	1:A:345:PRO:HD2	1.62	0.80
1:A:241:ARG:HD2	3:A:500:HOH:O	1.81	0.79
1:A:186:GLU:CD	1:A:186:GLU:H	1.87	0.78
1:A:4:ASP:O	1:A:8:VAL:HG23	1.84	0.77
1:A:225:LEU:HB3	1:A:228:GLN:HG3	1.67	0.77
1:A:373:GLU:CA	1:A:377:LYS:HD2	2.14	0.76
1:A:171:ILE:CG2	1:A:172:LEU:N	2.49	0.75
1:A:392:ARG:HH11	1:A:392:ARG:HG2	1.51	0.75
1:A:156:ALA:HB1	1:A:159:THR:HB	1.70	0.74
1:A:171:ILE:O	1:A:172:LEU:HD23	1.88	0.74
1:A:235:ARG:HG2	1:A:267:ALA:HB1	1.70	0.73
1:A:317:LYS:HG2	1:A:345:PRO:C	2.11	0.71
1:A:18:LEU:HD23	1:A:18:LEU:O	1.89	0.71
1:A:392:ARG:O	1:A:396:VAL:HG23	1.92	0.68
1:A:241:ARG:NH1	3:A:500:HOH:O	2.25	0.68
1:A:196:THR:HG22	1:A:201:VAL:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:HA	1:A:377:LYS:HB2	1.76	0.66
1:A:310:ALA:HB1	1:A:396:VAL:HG11	1.78	0.66
1:A:373:GLU:HA	1:A:377:LYS:CD	2.25	0.65
1:A:375:LEU:HD12	1:A:375:LEU:N	2.12	0.65
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.11	0.65
1:A:255:PRO:HD2	1:A:256:HIS:CE1	2.32	0.64
1:A:225:LEU:O	1:A:228:GLN:HB2	1.98	0.64
1:A:373:GLU:N	1:A:377:LYS:HD2	2.13	0.64
1:A:189:ARG:HD2	1:A:190:LYS:HE3	1.81	0.63
1:A:336:ALA:O	1:A:339:ILE:HG22	1.98	0.63
1:A:330:LEU:HA	1:A:333:GLU:OE2	1.98	0.62
1:A:373:GLU:HA	1:A:377:LYS:CB	2.30	0.62
1:A:229:ASN:HD22	1:A:229:ASN:C	2.04	0.61
1:A:75:LYS:HB3	1:A:77:VAL:HG13	1.83	0.61
1:A:54:SER:OG	1:A:57:ILE:HG12	2.01	0.61
1:A:73:ASN:HB3	1:A:84:ALA:O	2.01	0.61
1:A:173:GLU:HG2	1:A:192:VAL:CG2	2.28	0.61
1:A:236:ARG:HE	1:A:237:ASN:ND2	2.00	0.60
1:A:143:HIS:HB3	1:A:145:LEU:HD13	1.83	0.60
1:A:381:GLU:HA	1:A:384:ARG:HD2	1.83	0.60
1:A:339:ILE:HG13	1:A:340:LEU:N	2.17	0.59
1:A:189:ARG:HB3	1:A:190:LYS:HD2	1.85	0.58
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.68	0.58
1:A:72:PHE:O	1:A:74:LYS:HD3	2.03	0.58
1:A:41:THR:CB	1:A:84:ALA:HB1	2.34	0.58
1:A:4:ASP:C	1:A:7:GLY:H	2.06	0.58
1:A:134:LEU:HD23	1:A:386:THR:CG2	2.33	0.58
1:A:314:PHE:HB3	1:A:340:LEU:HB2	1.85	0.58
1:A:19:LEU:O	1:A:22:MET:HB2	2.04	0.57
1:A:317:LYS:HA	1:A:345:PRO:HA	1.84	0.57
1:A:109:PRO:CD	1:A:246:TYR:O	2.53	0.57
1:A:185:ALA:HB3	1:A:186:GLU:OE2	2.04	0.57
1:A:286:LEU:O	1:A:290:THR:HG22	2.03	0.57
1:A:229:ASN:HD22	1:A:231:TYR:N	1.98	0.57
1:A:305:GLU:N	1:A:305:GLU:CD	2.58	0.57
1:A:344:LEU:HB2	1:A:385:PHE:CE1	2.40	0.57
1:A:41:THR:HB	1:A:84:ALA:HB1	1.88	0.56
1:A:109:PRO:HD2	1:A:246:TYR:O	2.06	0.56
1:A:235:ARG:HG2	1:A:267:ALA:CB	2.36	0.56
1:A:134:LEU:HD23	1:A:386:THR:HG22	1.87	0.55
1:A:137:HIS:O	1:A:141:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HE	1:A:237:ASN:HD21	1.54	0.55
1:A:334:VAL:HG23	1:A:335:TYR:N	2.18	0.55
1:A:158:SER:O	1:A:161:PHE:HD1	1.89	0.55
1:A:225:LEU:HB3	1:A:228:GLN:CG	2.37	0.54
1:A:385:PHE:O	1:A:389:VAL:HG23	2.07	0.54
1:A:143:HIS:CB	1:A:145:LEU:HD13	2.37	0.54
1:A:45:ASN:O	1:A:49:LYS:HG3	2.08	0.54
1:A:105:ILE:HD12	1:A:105:ILE:N	2.22	0.54
1:A:171:ILE:HG21	1:A:205:PRO:HG3	1.90	0.54
1:A:332:ARG:HD3	1:A:339:ILE:HG21	1.89	0.54
1:A:228:GLN:HE21	1:A:228:GLN:CA	2.20	0.54
1:A:392:ARG:NH1	1:A:392:ARG:HG2	2.22	0.54
1:A:150:ILE:HG12	1:A:204:ILE:HD12	1.89	0.53
1:A:379:ARG:O	1:A:383:GLU:HG3	2.08	0.53
1:A:156:ALA:HB1	1:A:159:THR:CB	2.38	0.53
1:A:330:LEU:O	1:A:333:GLU:HB2	2.09	0.53
1:A:389:VAL:O	1:A:393:ILE:HD13	2.08	0.53
1:A:94:TYR:HD2	1:A:99:ILE:HD12	1.74	0.53
1:A:115:VAL:HG12	1:A:115:VAL:O	2.09	0.52
1:A:218:ARG:O	1:A:222:GLU:HG3	2.08	0.52
1:A:287:LYS:O	1:A:290:THR:CG2	2.57	0.52
1:A:318:MET:SD	1:A:328:HIS:ND1	2.82	0.52
1:A:102:TYR:CZ	1:A:106:HIS:CD2	2.98	0.52
1:A:271:LEU:HB2	1:A:308:LEU:HD11	1.91	0.52
1:A:179:MET:HE3	1:A:234:LEU:HB2	1.92	0.52
1:A:186:GLU:CD	1:A:186:GLU:N	2.61	0.52
1:A:51:PRO:CG	1:A:139:ASP:HB3	2.37	0.52
1:A:186:GLU:HA	1:A:190:LYS:HZ2	1.75	0.52
1:A:197:ILE:HG13	1:A:198:VAL:HG23	1.92	0.51
1:A:317:LYS:N	1:A:344:LEU:O	2.24	0.51
1:A:218:ARG:NH1	1:A:222:GLU:OE2	2.44	0.51
1:A:305:GLU:H	1:A:305:GLU:CD	2.14	0.51
1:A:319:THR:OG1	1:A:321:LYS:HE2	2.11	0.51
1:A:380:THR:HG22	1:A:384:ARG:CZ	2.41	0.51
1:A:9:GLY:O	1:A:12:ALA:HB3	2.11	0.51
1:A:77:VAL:HG22	1:A:82:GLN:CG	2.41	0.50
1:A:88:GLN:HB2	3:A:504:HOH:O	2.12	0.50
1:A:344:LEU:HB2	1:A:385:PHE:CZ	2.47	0.50
1:A:188:LEU:HA	1:A:192:VAL:HB	1.94	0.50
1:A:109:PRO:HG3	1:A:243:ALA:HA	1.94	0.50
1:A:117:LEU:HD23	1:A:117:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:HB2	1:A:339:ILE:HB	1.93	0.50
1:A:102:TYR:HB2	1:A:143:HIS:HB3	1.92	0.49
1:A:285:THR:O	1:A:289:LEU:HG	2.11	0.49
1:A:289:LEU:C	1:A:291:ARG:H	2.16	0.49
1:A:126:SER:O	1:A:129:THR:N	2.45	0.49
1:A:258:ASP:O	1:A:259:PRO:C	2.50	0.49
1:A:277:PRO:HD3	1:A:316:SER:O	2.13	0.49
1:A:382:ALA:O	1:A:385:PHE:HB3	2.13	0.49
1:A:18:LEU:HD23	1:A:18:LEU:C	2.32	0.49
1:A:317:LYS:O	1:A:318:MET:C	2.52	0.48
1:A:126:SER:O	1:A:129:THR:HB	2.13	0.48
1:A:16:SER:O	1:A:19:LEU:HB2	2.14	0.47
1:A:112:ILE:HG12	1:A:270:LEU:HD12	1.96	0.47
1:A:272:LEU:HD23	1:A:272:LEU:C	2.34	0.47
1:A:109:PRO:CG	1:A:243:ALA:HA	2.44	0.47
1:A:299:LEU:O	1:A:304:VAL:HG13	2.13	0.47
1:A:57:ILE:HG23	1:A:97:ARG:CZ	2.44	0.47
1:A:278:ALA:HB3	1:A:281:ASP:HB2	1.97	0.47
1:A:236:ARG:HH21	1:A:237:ASN:HD21	1.62	0.47
1:A:155:GLN:OE1	1:A:155:GLN:N	2.48	0.47
1:A:105:ILE:CD1	1:A:105:ILE:N	2.78	0.47
1:A:132:HIS:NE2	1:A:196:THR:HG21	2.30	0.47
1:A:214:ALA:O	1:A:216:GLN:N	2.48	0.47
1:A:273:THR:O	1:A:313:GLY:HA2	2.16	0.46
1:A:373:GLU:HA	1:A:377:LYS:CG	2.46	0.46
1:A:341:ASP:CG	1:A:392:ARG:HH22	2.19	0.46
1:A:229:ASN:ND2	1:A:229:ASN:C	2.68	0.46
1:A:158:SER:O	1:A:160:MET:N	2.49	0.46
1:A:385:PHE:O	1:A:388:ALA:HB3	2.16	0.45
1:A:108:SER:O	1:A:109:PRO:HB2	2.16	0.45
1:A:189:ARG:HD2	1:A:190:LYS:CE	2.46	0.45
1:A:307:ARG:NH2	3:A:529:HOH:O	2.50	0.45
1:A:43:THR:HG22	1:A:44:ARG:N	2.30	0.45
1:A:109:PRO:HD3	1:A:246:TYR:O	2.15	0.45
1:A:171:ILE:HD13	1:A:205:PRO:CB	2.46	0.45
1:A:322:ARG:O	1:A:326:THR:N	2.50	0.45
1:A:310:ALA:CB	1:A:396:VAL:HG11	2.45	0.45
1:A:175:ALA:O	1:A:179:MET:HG3	2.17	0.45
1:A:287:LYS:O	1:A:290:THR:HG22	2.17	0.45
1:A:392:ARG:NH1	1:A:392:ARG:CG	2.80	0.45
1:A:214:ALA:C	1:A:216:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:H	1:A:259:PRO:HD2	1.82	0.44
1:A:82:GLN:HB3	1:A:83:TYR:H	1.50	0.44
1:A:181:ASN:O	1:A:182:ASN:C	2.56	0.44
1:A:375:LEU:CD1	1:A:375:LEU:N	2.81	0.44
1:A:235:ARG:NH2	3:A:529:HOH:O	2.45	0.44
1:A:228:GLN:HE21	1:A:228:GLN:HA	1.82	0.44
1:A:47:VAL:O	1:A:50:LEU:HB2	2.17	0.44
1:A:373:GLU:CA	1:A:377:LYS:HB2	2.47	0.44
1:A:104:ASP:C	1:A:105:ILE:HD12	2.38	0.44
1:A:344:LEU:HD12	1:A:345:PRO:CD	2.39	0.44
1:A:41:THR:OG1	1:A:84:ALA:HB1	2.18	0.43
1:A:275:THR:O	1:A:315:MET:HA	2.17	0.43
1:A:190:LYS:HD2	1:A:190:LYS:H	1.83	0.43
1:A:253:THR:HG22	1:A:254:GLY:N	2.33	0.43
1:A:282:PHE:CG	1:A:327:SER:HB2	2.54	0.43
1:A:228:GLN:HA	1:A:228:GLN:NE2	2.33	0.43
1:A:287:LYS:O	1:A:290:THR:HG23	2.18	0.43
1:A:77:VAL:HG22	1:A:82:GLN:HG2	2.00	0.43
1:A:304:VAL:HG23	1:A:305:GLU:N	2.34	0.42
1:A:60:GLN:O	1:A:64:GLU:HG3	2.18	0.42
1:A:397:ARG:HD2	2:A:598:SO4:O4	2.19	0.42
1:A:87:ILE:O	1:A:91:ILE:HG13	2.20	0.42
1:A:4:ASP:OD1	1:A:7:GLY:C	2.57	0.42
1:A:52:LYS:O	1:A:53:LEU:HD23	2.19	0.42
1:A:270:LEU:HD21	1:A:312:ILE:HG12	2.01	0.42
1:A:335:TYR:O	1:A:338:ASN:HB2	2.19	0.42
1:A:51:PRO:HG2	1:A:139:ASP:CB	2.43	0.42
1:A:256:HIS:O	1:A:257:LEU:C	2.58	0.42
1:A:314:PHE:CZ	1:A:385:PHE:HZ	2.37	0.42
1:A:190:LYS:HD2	1:A:190:LYS:N	2.35	0.42
1:A:171:ILE:HD13	1:A:205:PRO:HB3	2.01	0.41
1:A:171:ILE:HG21	1:A:205:PRO:CG	2.51	0.41
1:A:326:THR:O	1:A:330:LEU:HG	2.21	0.41
1:A:270:LEU:HD22	1:A:271:LEU:N	2.36	0.41
1:A:96:HIS:C	1:A:98:LYS:H	2.23	0.41
1:A:225:LEU:HD13	1:A:233:ILE:HD12	2.03	0.41
1:A:149:VAL:O	1:A:203:VAL:HG13	2.20	0.41
1:A:297:GLU:O	1:A:300:GLU:HB2	2.21	0.40
1:A:66:GLU:HA	1:A:69:GLY:O	2.20	0.40
1:A:384:ARG:H	1:A:384:ARG:HG2	1.69	0.40
1:A:323:ASP:HA	1:A:326:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG22	1:A:82:GLN:HG3	2.02	0.40
1:A:255:PRO:HB2	1:A:256:HIS:H	1.56	0.40
1:A:289:LEU:O	1:A:291:ARG:N	2.54	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)
1:A:5:TYR:OH	1:A:300:GLU:OE1[4_665]	2.18	0.02

## 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	332/403 (82%)	283 (85%)	34 (10%)	15 (4%)	<b>2</b> <b>8</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	TYR
1	A	109	PRO
1	A	70	TYR
1	A	79	ASN
1	A	159	THR
1	A	255	PRO
1	A	256	HIS
1	A	333	GLU
1	A	215	SER
1	A	258	ASP
1	A	290	THR
1	A	322	ARG
1	A	257	LEU

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Mol	Chain	Res	Type
1	A	39	TYR
1	A	334	VAL

### 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	296 / 350 (85%)	257 (87%)	39 (13%)	<b>4</b> <b>12</b>

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	39	TYR
1	A	50	LEU
1	A	63	LYS
1	A	67	GLU
1	A	71	GLN
1	A	76	GLN
1	A	83	TYR
1	A	97	ARG
1	A	108	SER
1	A	109	PRO
1	A	130	LEU
1	A	135	ARG
1	A	139	ASP
1	A	145	LEU
1	A	152	LEU
1	A	155	GLN
1	A	228	GLN
1	A	229	ASN
1	A	234	LEU
1	A	235	ARG
1	A	241	ARG
1	A	252	ASP
1	A	256	HIS

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Mol	Chain	Res	Type
1	A	257	LEU
1	A	258	ASP
1	A	261	LEU
1	A	269	ASP
1	A	270	LEU
1	A	279	GLN
1	A	281	ASP
1	A	291	ARG
1	A	304	VAL
1	A	305	GLU
1	A	333	GLU
1	A	342	SER
1	A	379	ARG
1	A	392	ARG
1	A	397	ARG

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	76	GLN
1	A	137	HIS
1	A	177	GLN
1	A	228	GLN
1	A	229	ASN
1	A	230	GLN
1	A	237	ASN
1	A	298	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	796	-	4,4,4	0.24	0	6,6,6	0.04	0
2	SO4	A	597	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	A	696	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	A	598	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	A	596	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	A	896	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	A	599	-	4,4,4	0.26	0	6,6,6	0.07	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	696	SO4	1	0
2	A	598	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, 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	342/403 (84%)	0.43	21 (6%) 21 13	30, 59, 101, 137	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	GLU	8.7
1	A	171	ILE	5.4
1	A	375	LEU	5.2
1	A	170	SER	5.1
1	A	377	LYS	5.0
1	A	399	GLU	4.9
1	A	345	PRO	4.3
1	A	381	GLU	3.1
1	A	331	ALA	3.1
1	A	4	ASP	3.0
1	A	327	SER	3.0
1	A	344	LEU	2.9
1	A	374	ALA	2.7
1	A	315	MET	2.7
1	A	326	THR	2.7
1	A	3	ARG	2.4
1	A	333	GLU	2.3
1	A	318	MET	2.3
1	A	117	LEU	2.1
1	A	169	GLY	2.0
1	A	282	PHE	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 carbohydrates 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	599	5/5	0.65	0.29	151,152,152,153	0
2	SO4	A	896	5/5	0.74	0.29	124,125,126,126	0
2	SO4	A	596	5/5	0.81	0.34	138,138,138,139	0
2	SO4	A	796	5/5	0.83	0.56	163,163,164,164	0
2	SO4	A	598	5/5	0.84	0.25	126,127,127,127	0
2	SO4	A	696	5/5	0.86	0.17	131,131,131,132	0
2	SO4	A	597	5/5	0.89	0.11	111,111,112,113	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.