



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:16 PM GMT

PDB ID : 1O57  
Title : CRYSTAL STRUCTURE OF THE PURINE OPERON REPRESSOR OF BACILLUS SUBTILIS  
Authors : Sinha, S.C.; Krahn, J.; Shin, B.S.; Tomchick, D.R.; Zalkin, H.; Smith, J.L.  
Deposited on : 2003-04-20  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

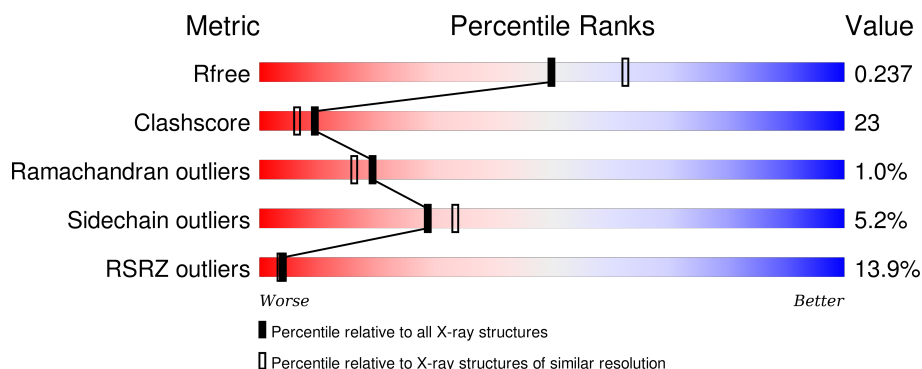
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	291	
1	B	291	
1	C	291	
1	D	291	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	589	-	-	-	X
2	SO4	C	590	-	-	-	X
3	EPE	A	570	-	-	-	X
3	EPE	D	571	-	-	-	X
4	P6G	A	572	-	-	-	X
4	P6G	D	573	-	-	-	X
5	2PE	A	574	-	-	-	X
6	PG4	B	575	-	-	-	X
7	1PE	C	576	-	-	-	X
7	1PE	D	577	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9132 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 PUR OPERON REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	8	0
			2099	1338	347	400	14			
1	B	269	Total	C	N	O	S	0	8	0
			2091	1334	346	397	14			
1	C	269	Total	C	N	O	S	0	9	0
			2097	1340	346	395	16			
1	D	270	Total	C	N	O	S	0	7	0
			2096	1337	346	399	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	HIS	-	EXPRESSION TAG	UNP P37551
A	287	HIS	-	EXPRESSION TAG	UNP P37551
A	288	HIS	-	EXPRESSION TAG	UNP P37551
A	289	HIS	-	EXPRESSION TAG	UNP P37551
A	290	HIS	-	EXPRESSION TAG	UNP P37551
A	291	HIS	-	EXPRESSION TAG	UNP P37551
B	286	HIS	-	EXPRESSION TAG	UNP P37551
B	287	HIS	-	EXPRESSION TAG	UNP P37551
B	288	HIS	-	EXPRESSION TAG	UNP P37551
B	289	HIS	-	EXPRESSION TAG	UNP P37551
B	290	HIS	-	EXPRESSION TAG	UNP P37551
B	291	HIS	-	EXPRESSION TAG	UNP P37551
C	286	HIS	-	EXPRESSION TAG	UNP P37551
C	287	HIS	-	EXPRESSION TAG	UNP P37551
C	288	HIS	-	EXPRESSION TAG	UNP P37551
C	289	HIS	-	EXPRESSION TAG	UNP P37551
C	290	HIS	-	EXPRESSION TAG	UNP P37551
C	291	HIS	-	EXPRESSION TAG	UNP P37551
D	286	HIS	-	EXPRESSION TAG	UNP P37551
D	287	HIS	-	EXPRESSION TAG	UNP P37551
D	288	HIS	-	EXPRESSION TAG	UNP P37551

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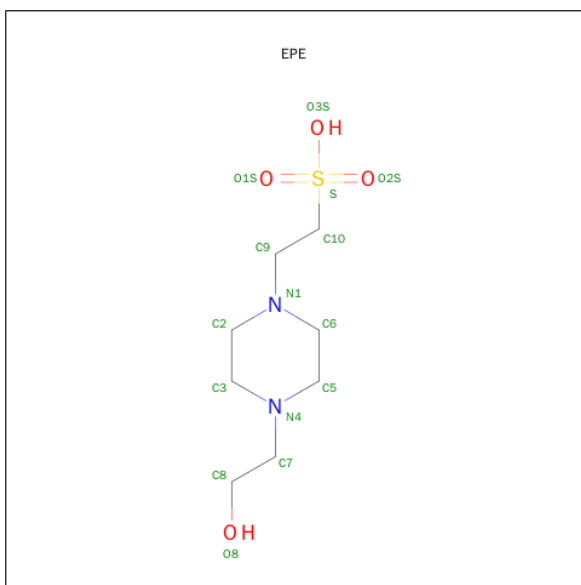
Chain	Residue	Modelled	Actual	Comment	Reference
D	289	HIS	-	EXPRESSION TAG	UNP P37551
D	290	HIS	-	EXPRESSION TAG	UNP P37551
D	291	HIS	-	EXPRESSION TAG	UNP P37551

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



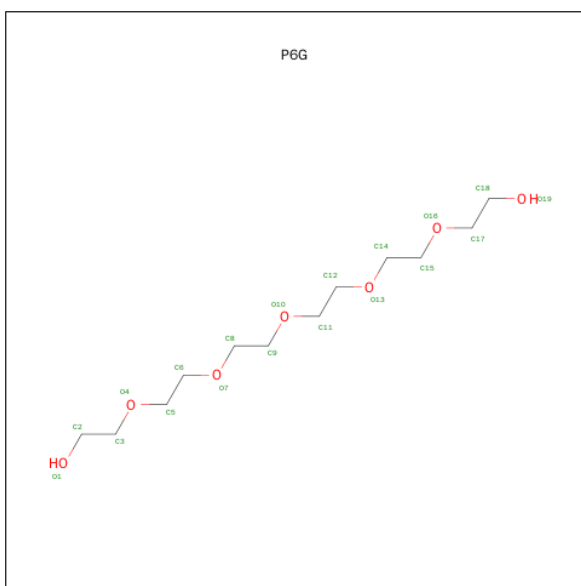
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



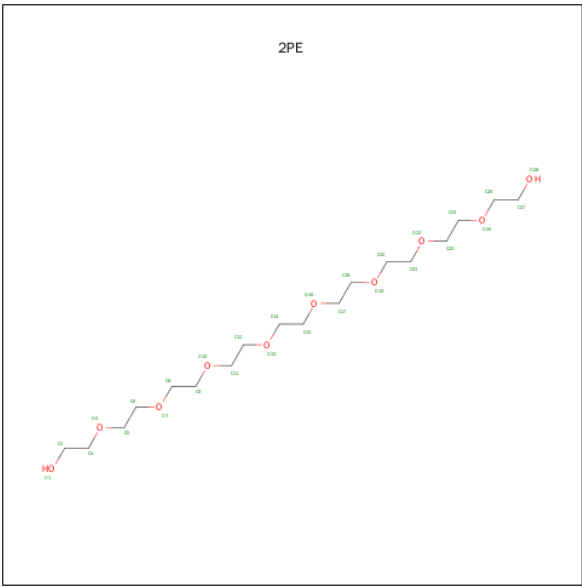
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 8	N 2	O 4	S 1	0	0
3	D	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $\text{C}_{12}\text{H}_{26}\text{O}_7$ ).



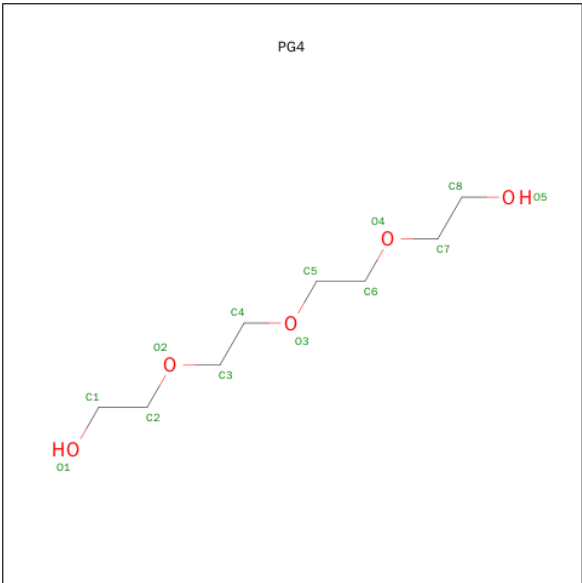
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		
4	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



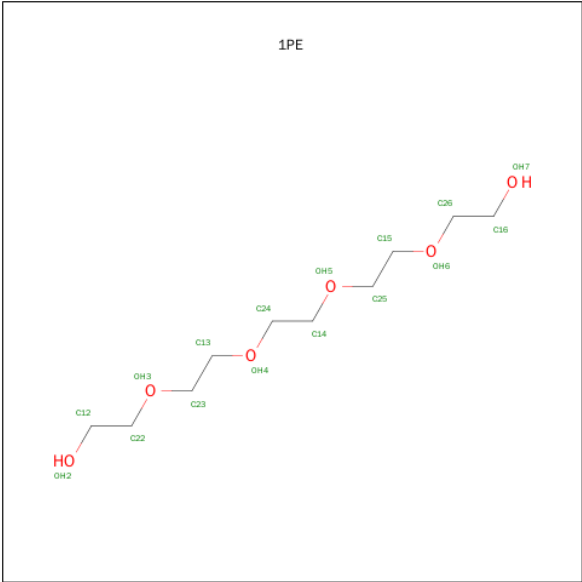
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			28	18	10		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	10	6		
7	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

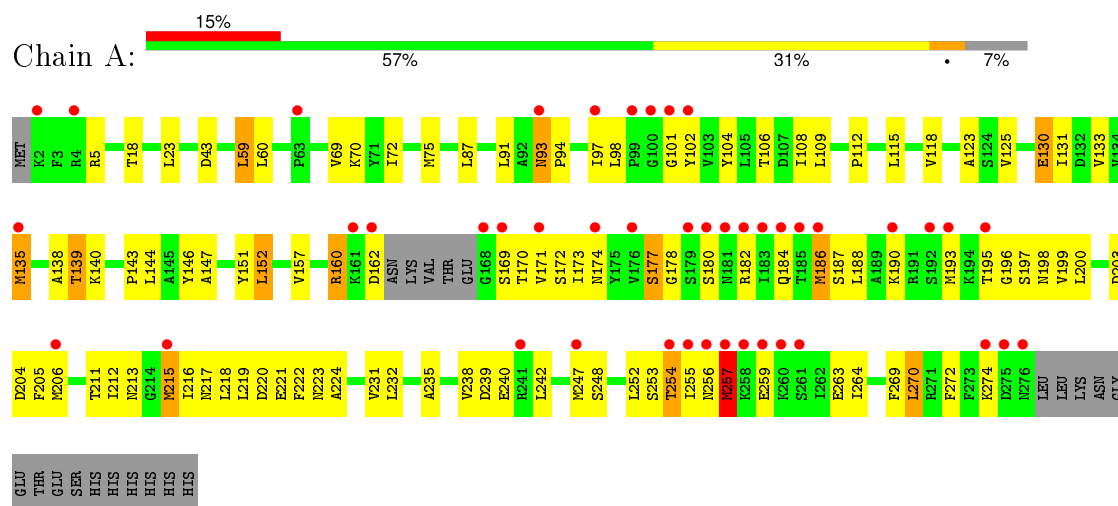
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	121	Total	O	0	0
			121	121		
8	B	138	Total	O	0	0
			138	138		
8	C	177	Total	O	0	0
			177	177		
8	D	132	Total	O	0	0
			132	132		



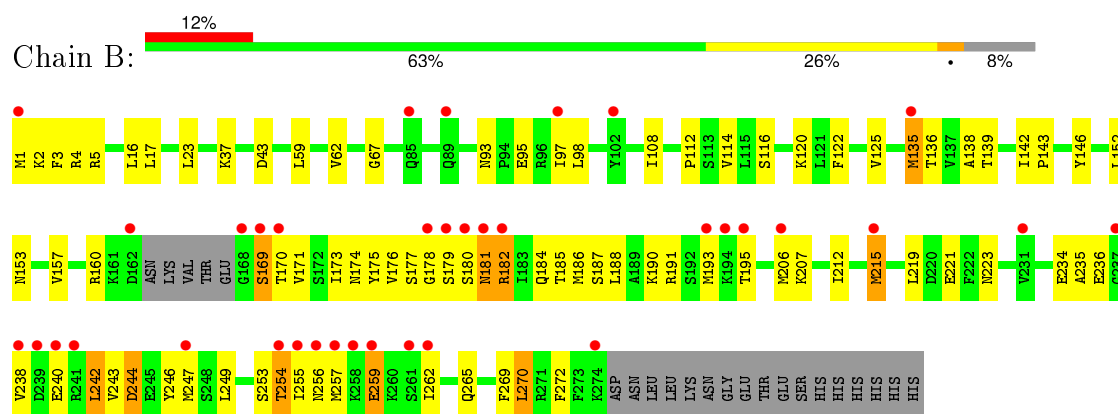
### 3 Residue-property plots

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.

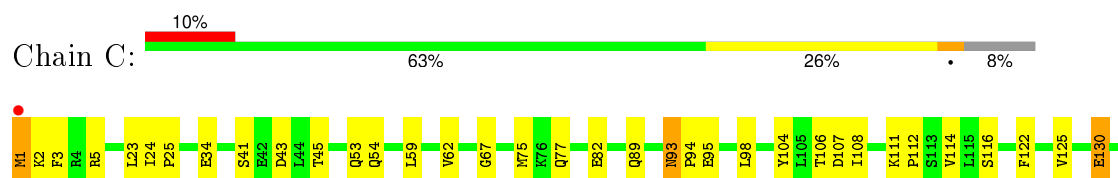
#### • Molecule 1: PUR OPERON REPRESSOR

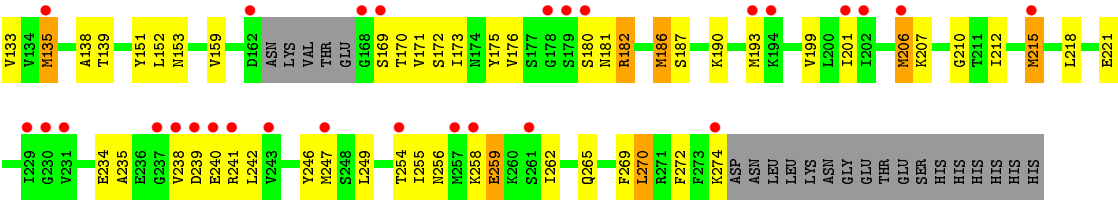


#### • Molecule 1: PUR OPERON REPRESSOR

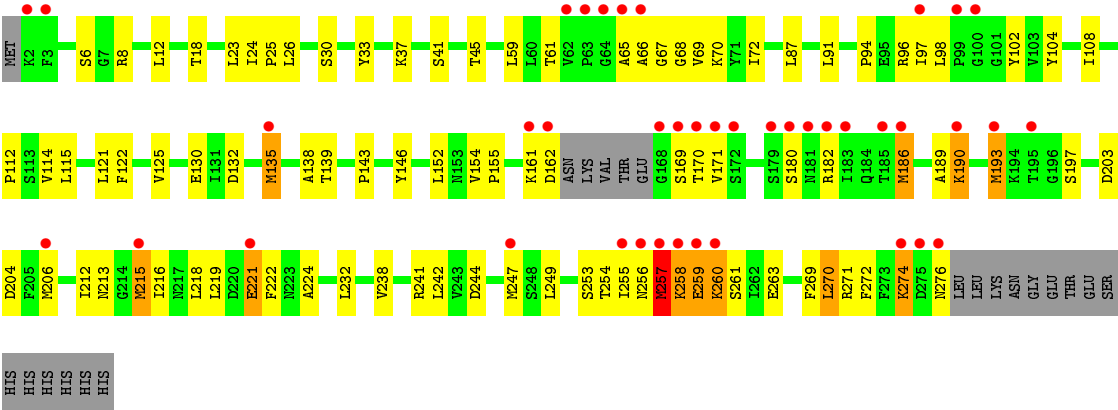


#### • Molecule 1: PUR OPERON REPRESSOR





● Molecule 1: PUR OPERON REPRESSOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.08Å 72.16Å 82.97Å 84.75° 84.03° 67.47°	Depositor
Resolution (Å)	20.00 – 2.20 27.68 – 2.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.20) 91.8 (27.68-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.188 , 0.237 0.194 , 0.237	Depositor DCC
$R_{free}$ test set	3330 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 70732 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 1PE, PG4, 2PE, SO4, P6G, EPE

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	0.69	10/2169 (0.5%)	0.70	0/2924
1	B	0.70	7/2162 (0.3%)	0.71	0/2914
1	C	0.76	10/2173 (0.5%)	0.74	0/2926
1	D	0.69	9/2161 (0.4%)	0.72	0/2913
All	All	0.71	36/8665 (0.4%)	0.72	0/11677

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	135[A]	MET	CG-SD	7.06	1.99	1.81
1	C	135[B]	MET	CG-SD	7.06	1.99	1.81
1	B	135[A]	MET	CG-SD	6.59	1.98	1.81
1	B	135[B]	MET	CG-SD	6.59	1.98	1.81
1	D	215[A]	MET	CG-SD	6.59	1.98	1.81
1	D	215[B]	MET	CG-SD	6.59	1.98	1.81
1	C	75	MET	CG-SD	6.25	1.97	1.81
1	B	215[A]	MET	CG-SD	6.07	1.97	1.81
1	B	215[B]	MET	CG-SD	6.07	1.97	1.81
1	C	206[A]	MET	CG-SD	6.03	1.96	1.81
1	C	206[B]	MET	CG-SD	6.03	1.96	1.81
1	A	75	MET	CG-SD	5.99	1.96	1.81
1	A	206[A]	MET	CG-SD	5.95	1.96	1.81
1	A	206[B]	MET	CG-SD	5.95	1.96	1.81
1	A	135[A]	MET	CG-SD	5.87	1.96	1.81
1	A	135[B]	MET	CG-SD	5.87	1.96	1.81
1	B	186	MET	CG-SD	5.85	1.96	1.81
1	C	186[A]	MET	CG-SD	5.79	1.96	1.81
1	C	186[B]	MET	CG-SD	5.79	1.96	1.81
1	D	135[A]	MET	CG-SD	5.70	1.96	1.81
1	D	135[B]	MET	CG-SD	5.70	1.96	1.81
1	A	257	MET	CG-SD	5.70	1.96	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CG-SD	5.69	1.96	1.81
1	D	186[A]	MET	CG-SD	5.62	1.95	1.81
1	D	186[B]	MET	CG-SD	5.62	1.95	1.81
1	A	215[A]	MET	CG-SD	5.57	1.95	1.81
1	A	215[B]	MET	CG-SD	5.57	1.95	1.81
1	A	186[A]	MET	CG-SD	5.46	1.95	1.81
1	A	186[B]	MET	CG-SD	5.46	1.95	1.81
1	D	257	MET	CG-SD	5.42	1.95	1.81
1	D	193[A]	MET	CG-SD	5.39	1.95	1.81
1	D	193[B]	MET	CG-SD	5.39	1.95	1.81
1	B	257	MET	CG-SD	5.26	1.94	1.81
1	C	1	MET	CG-SD	5.12	1.94	1.81
1	C	215[A]	MET	CG-SD	5.01	1.94	1.81
1	C	215[B]	MET	CG-SD	5.01	1.94	1.81

There are no bond angle outliers.

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	2099	0	2164	105	0
1	B	2091	0	2161	79	0
1	C	2097	0	2177	102	0
1	D	2096	0	2162	106	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	17	3	0
3	D	15	0	17	1	0
4	A	19	0	26	2	0
4	D	19	0	26	2	0
5	A	28	0	38	10	0
6	B	13	0	18	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	16	0	22	5	0
7	D	16	0	22	4	0
8	A	121	0	0	1	0
8	B	138	0	0	7	0
8	C	177	0	0	6	0
8	D	132	0	0	7	0
All	All	9132	0	8850	395	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 23.

All (395) 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:97:ILE:HG22	1:A:255:ILE:HD11	1.32	1.12
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.18	1.04
1:B:182:ARG:HG2	1:B:182:ARG:NH1	1.86	0.88
1:B:178:GLY:C	1:B:180:SER:H	1.78	0.87
1:D:190:LYS:HA	1:D:190:LYS:NZ	1.93	0.83
1:C:201:ILE:HG23	1:C:215[A]:MET:HE2	1.57	0.83
1:A:101:GLY:HA2	1:A:255:ILE:HG22	1.58	0.83
1:C:201:ILE:HG23	1:C:215[A]:MET:CE	2.08	0.82
1:D:97:ILE:HG12	1:D:255:ILE:HD11	1.62	0.82
1:C:135[A]:MET:HG2	1:C:215[A]:MET:HE3	1.62	0.81
1:B:138:ALA:HB1	1:B:139:THR:HG22	1.63	0.80
1:D:41:SER:O	1:D:45:THR:HG23	1.79	0.80
1:A:94:PRO:O	1:A:97:ILE:HG13	1.83	0.78
1:A:235:ALA:O	1:A:238:VAL:HG23	1.83	0.78
1:B:97:ILE:HG23	1:B:255:ILE:HD11	1.65	0.78
1:A:193[A]:MET:CE	1:A:197:SER:HB2	2.13	0.78
1:A:253:SER:HB2	1:A:263:GLU:HB2	1.66	0.78
1:C:256:ASN:HD21	1:C:259:GLU:CD	1.87	0.78
1:D:190:LYS:HA	1:D:190:LYS:HZ3	1.46	0.77
1:D:271:ARG:HD2	8:D:703:HOH:O	1.83	0.76
1:B:182:ARG:HA	8:B:694:HOH:O	1.84	0.76
1:C:2:LYS:NZ	1:C:2:LYS:HB3	2.01	0.76
1:B:243:VAL:HG13	1:B:244:ASP:OD2	1.87	0.75
1:C:258:LYS:HB3	1:C:259:GLU:OE1	1.86	0.75
1:B:182:ARG:CG	1:B:182:ARG:HH11	1.99	0.75
1:C:172:SER:O	1:C:173:ILE:HD12	1.87	0.75
1:B:236:GLU:HG2	8:B:704:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:HD22	1:C:94:PRO:CD	2.01	0.73
1:C:125:VAL:HG21	1:C:247[A]:MET:HE2	1.71	0.73
1:A:125:VAL:HG21	1:A:247[A]:MET:HE2	1.68	0.72
1:D:190:LYS:HA	1:D:190:LYS:CE	2.20	0.71
1:A:147:ALA:HB2	5:A:574:2PE:H52	1.70	0.71
1:D:244:ASP:HB3	8:D:597:HOH:O	1.91	0.71
1:B:256:ASN:ND2	1:B:259:GLU:HB2	2.05	0.70
1:D:97:ILE:HG23	1:D:255:ILE:HD11	1.73	0.70
1:A:93:ASN:HD22	1:A:94:PRO:HD2	1.57	0.70
1:C:256:ASN:HD22	1:C:259:GLU:HB2	1.57	0.69
1:D:70:LYS:HD3	1:D:72:ILE:HD11	1.74	0.69
1:C:135[A]:MET:HG2	1:C:215[A]:MET:CE	2.22	0.69
1:C:207:LYS:O	1:C:238:VAL:HG12	1.92	0.69
1:B:182:ARG:NH1	1:C:130:GLU:OE2	2.26	0.69
1:C:138:ALA:HB1	1:C:139:THR:HG22	1.74	0.68
1:A:169:SER:O	1:A:190:LYS:HB2	1.93	0.68
1:B:253:SER:OG	1:B:265[A]:GLN:NE2	2.20	0.68
1:C:2:LYS:HE2	1:C:34:GLU:O	1.93	0.68
1:A:97:ILE:O	1:A:97:ILE:HD12	1.95	0.67
1:B:178:GLY:O	1:B:180:SER:N	2.27	0.67
1:A:212:ILE:O	1:A:216:ILE:HG13	1.94	0.67
1:C:133:VAL:HG11	1:C:193[B]:MET:HE2	1.78	0.66
1:A:193[A]:MET:HE3	1:A:197:SER:HB2	1.77	0.66
1:C:93:ASN:HD22	1:C:94:PRO:HD2	1.59	0.66
1:D:171:VAL:HG23	1:D:190:LYS:CE	2.26	0.66
1:D:212:ILE:O	1:D:216:ILE:HG13	1.96	0.66
1:A:91:LEU:HD21	1:A:108:ILE:HD13	1.77	0.66
1:A:193[A]:MET:HE1	1:A:197:SER:HB2	1.77	0.65
1:C:255:ILE:N	8:C:741:HOH:O	2.23	0.65
1:C:93:ASN:HD22	1:C:94:PRO:N	1.95	0.65
1:D:108:ILE:HG23	1:D:114:VAL:HG11	1.78	0.65
1:C:201:ILE:CG2	1:C:215[A]:MET:HE2	2.27	0.65
6:B:575:PG4:H32	8:B:659:HOH:O	1.98	0.64
1:C:207:LYS:O	1:C:238:VAL:CG1	2.46	0.64
1:D:26:LEU:HD22	1:D:68:GLY:HA2	1.79	0.64
1:D:190:LYS:CA	1:D:190:LYS:CE	2.75	0.64
1:C:135[A]:MET:CG	1:C:215[A]:MET:HE3	2.26	0.64
1:C:256:ASN:ND2	1:C:259:GLU:CD	2.49	0.64
1:D:171:VAL:HB	1:D:190:LYS:HE3	1.81	0.63
1:D:23:LEU:HB2	4:D:573:P6G:H122	1.80	0.63
1:D:125:VAL:HG21	1:D:247[A]:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:HG12	1:B:255:ILE:HD11	1.80	0.63
1:D:169:SER:O	1:D:190:LYS:HD2	1.99	0.63
1:A:213:ASN:HD22	1:A:242:LEU:HD12	1.63	0.63
1:B:269:PHE:CE1	1:B:270:LEU:HD13	2.34	0.63
1:C:133:VAL:HG11	1:C:193[B]:MET:CE	2.28	0.63
1:D:213:ASN:HD22	1:D:242:LEU:HD12	1.64	0.63
1:A:101:GLY:HA2	1:A:255:ILE:CG2	2.28	0.63
1:C:235:ALA:O	1:C:238:VAL:HG13	1.98	0.63
1:C:269:PHE:CE1	1:C:270:LEU:HD13	2.34	0.63
1:B:4:ARG:HG2	1:B:4:ARG:HH11	1.64	0.62
5:A:574:2PE:H91	5:A:574:2PE:H151	1.79	0.62
1:A:98:LEU:HB2	1:A:102:TYR:O	2.00	0.62
1:A:93:ASN:HD22	1:A:94:PRO:CD	2.13	0.62
1:A:219:LEU:HB3	1:A:224:ALA:HB3	1.80	0.62
1:C:93:ASN:C	1:C:93:ASN:HD22	2.02	0.62
1:B:247[B]:MET:HE1	1:B:249:LEU:HD23	1.82	0.62
1:A:213:ASN:HD22	1:A:242:LEU:CD1	2.13	0.62
1:D:171:VAL:CB	1:D:190:LYS:HE3	2.30	0.62
1:C:53:GLN:HG2	1:C:54:GLN:HE21	1.64	0.61
1:D:190:LYS:N	1:D:190:LYS:HE2	2.14	0.61
1:C:180:SER:OG	1:C:182:ARG:HD3	2.00	0.61
1:A:97:ILE:O	1:A:98:LEU:HD12	1.99	0.61
1:C:112:PRO:HA	7:C:576:1PE:H222	1.82	0.61
1:D:18:THR:HA	7:D:577:1PE:H242	1.83	0.61
1:D:97:ILE:HG23	1:D:255:ILE:CD1	2.31	0.61
1:A:205:PHE:O	3:A:570:EPE:H72	2.00	0.61
1:B:169:SER:O	1:B:190:LYS:HB2	2.01	0.60
1:A:256:ASN:HA	1:A:257:MET:CE	2.32	0.60
1:C:247[B]:MET:HG3	1:C:272:PHE:CD1	2.37	0.60
1:D:26:LEU:CD2	1:D:68:GLY:HA2	2.32	0.60
1:D:169:SER:HB2	1:D:190:LYS:HB2	1.84	0.60
1:C:180:SER:C	1:C:182:ARG:H	2.04	0.60
1:C:2:LYS:HB3	1:C:2:LYS:HZ3	1.67	0.60
1:A:247[B]:MET:HG3	1:A:272:PHE:CD1	2.36	0.59
1:C:256:ASN:ND2	1:C:259:GLU:H	2.00	0.59
1:B:247[B]:MET:HG3	1:B:272:PHE:CD1	2.37	0.59
1:B:195:THR:HG23	1:B:223:ASN:HB2	1.83	0.59
1:C:170:THR:CG2	1:C:187:SER:HB2	2.31	0.59
1:B:206[A]:MET:CE	1:B:212:ILE:HD12	2.32	0.59
1:B:247[B]:MET:CE	1:B:249:LEU:HD23	2.33	0.59
1:D:94:PRO:O	1:D:97:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HD3	1:A:72:ILE:HD11	1.84	0.59
1:C:173:ILE:HD13	1:C:218:LEU:HD13	1.85	0.59
1:C:93:ASN:ND2	1:C:95:GLU:H	2.00	0.59
1:D:256:ASN:O	1:D:259:GLU:O	2.20	0.59
1:C:125:VAL:HG21	1:C:247[A]:MET:CE	2.32	0.59
1:D:257:MET:HB3	8:D:705:HOH:O	2.02	0.58
1:B:174:ASN:OD1	1:B:185:THR:HG22	2.03	0.58
1:A:139:THR:HG21	1:B:160:ARG:HH22	1.68	0.58
1:A:70:LYS:CD	1:A:72:ILE:HD11	2.33	0.58
1:A:125:VAL:HG21	1:A:247[A]:MET:CE	2.33	0.58
1:B:170:THR:CG2	1:B:187:SER:HB2	2.33	0.58
1:B:170:THR:HG21	1:B:187:SER:HB2	1.84	0.58
1:D:218:LEU:HD23	1:D:218:LEU:O	2.04	0.58
1:B:247[B]:MET:HE1	1:B:249:LEU:CD2	2.32	0.58
7:D:577:1PE:H122	7:D:577:1PE:H251	1.85	0.58
1:A:146:TYR:HB3	5:A:574:2PE:H82	1.84	0.57
1:B:108:ILE:HG23	1:B:114:VAL:HG11	1.87	0.57
1:A:135[B]:MET:HE1	1:A:219:LEU:HD11	1.85	0.56
1:A:135[A]:MET:SD	1:A:219:LEU:HD11	2.45	0.56
1:D:189:ALA:C	1:D:190:LYS:HE2	2.25	0.56
1:A:269:PHE:CE1	1:A:270:LEU:HD13	2.41	0.56
1:D:138:ALA:HB1	1:D:139:THR:HG22	1.88	0.56
1:A:213:ASN:ND2	1:A:242:LEU:HD12	2.21	0.56
1:D:259:GLU:O	1:D:261:SER:N	2.39	0.55
1:A:239:ASP:O	1:A:240:GLU:HG3	2.06	0.55
1:A:211:THR:O	1:A:215[A]:MET:HG3	2.06	0.55
1:B:135[B]:MET:HG2	1:B:215[B]:MET:CE	2.36	0.55
1:D:193[B]:MET:HE1	1:D:224:ALA:HB2	1.88	0.55
1:D:59:LEU:HD22	1:D:69:VAL:CG2	2.36	0.55
1:A:146:TYR:CB	5:A:574:2PE:H82	2.37	0.55
1:B:181:ASN:C	1:B:181:ASN:HD22	2.09	0.55
1:D:135[B]:MET:HG2	1:D:215[B]:MET:CE	2.37	0.54
1:D:269:PHE:CE1	1:D:270:LEU:HD13	2.42	0.54
1:C:201:ILE:HG23	1:C:215[A]:MET:HE1	1.88	0.54
1:C:169:SER:O	1:C:190:LYS:HB2	2.07	0.54
1:B:206[A]:MET:HE3	1:B:212:ILE:HD12	1.90	0.54
1:A:204:ASP:OD2	3:A:570:EPE:H51	2.07	0.54
1:C:256:ASN:ND2	1:C:259:GLU:OE2	2.40	0.54
5:A:574:2PE:H112	5:A:574:2PE:H172	1.88	0.54
1:D:26:LEU:HD21	8:D:697:HOH:O	2.07	0.54
1:C:135[A]:MET:SD	1:C:215[A]:MET:HE3	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:C	1:C:93:ASN:ND2	2.61	0.54
1:B:93:ASN:HD21	1:B:95:GLU:HB2	1.71	0.54
1:A:112:PRO:O	5:A:574:2PE:H21	2.08	0.54
1:C:206[B]:MET:HE1	1:C:246:TYR:CE1	2.43	0.53
1:D:190:LYS:CA	1:D:190:LYS:HZ3	2.20	0.53
1:B:235:ALA:O	1:B:238:VAL:HG13	2.08	0.53
1:A:190:LYS:HD3	1:A:190:LYS:O	2.09	0.53
1:D:274:LYS:C	1:D:276:ASN:H	2.11	0.53
1:C:77:GLN:H	1:C:274:LYS:HE3	1.74	0.53
1:D:171:VAL:HG23	1:D:190:LYS:HE3	1.91	0.53
1:B:177:SER:H	1:B:181:ASN:HD21	1.57	0.53
1:C:256:ASN:ND2	1:C:259:GLU:HB2	2.24	0.52
1:C:270:LEU:HB2	8:C:611:HOH:O	2.08	0.52
1:A:138:ALA:HB1	1:A:139:THR:HG22	1.91	0.52
1:A:196:GLY:HA2	1:A:223:ASN:O	2.09	0.52
1:D:125:VAL:HG11	1:D:247[A]:MET:HE2	1.92	0.52
1:A:5:ARG:NE	1:A:43:ASP:OD1	2.42	0.52
1:B:5:ARG:HD3	1:B:43:ASP:OD1	2.10	0.52
1:A:174:ASN:HA	1:A:184:GLN:O	2.09	0.52
1:D:130:GLU:OE2	1:D:130:GLU:HA	2.09	0.52
1:A:256:ASN:O	1:A:259:GLU:O	2.27	0.52
1:B:175:TYR:HB2	8:B:632:HOH:O	2.10	0.52
1:D:180:SER:OG	1:D:182:ARG:HG2	2.10	0.51
1:A:59:LEU:HD22	1:A:69:VAL:CG2	2.40	0.51
1:B:157:VAL:HG11	1:B:188:LEU:HD21	1.92	0.51
1:A:252:LEU:HD23	1:A:264:ILE:CD1	2.41	0.51
1:D:190:LYS:CA	1:D:190:LYS:HE2	2.40	0.51
1:C:173:ILE:HD11	1:C:221:GLU:HG3	1.92	0.51
1:A:256:ASN:HA	1:A:257:MET:HE3	1.92	0.51
1:A:135[B]:MET:CE	1:A:219:LEU:HD11	2.41	0.51
1:B:136:THR:C	1:B:215[B]:MET:HE3	2.30	0.51
1:D:171:VAL:CG2	1:D:190:LYS:HE3	2.40	0.51
1:D:65:ALA:O	1:D:66:ALA:HB3	2.11	0.51
1:D:97:ILE:CG1	1:D:255:ILE:HD11	2.38	0.50
1:C:116:SER:HA	7:C:576:1PE:H232	1.93	0.50
1:D:171:VAL:H	1:D:190:LYS:HE3	1.75	0.50
1:D:253:SER:O	1:D:255:ILE:N	2.45	0.50
1:B:136:THR:CA	1:B:215[B]:MET:HE3	2.42	0.50
1:D:258:LYS:C	1:D:258:LYS:HD3	2.31	0.50
1:C:5:ARG:HD3	1:C:43:ASP:OD1	2.12	0.50
1:D:213:ASN:HD22	1:D:242:LEU:CD1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:TYR:CZ	7:C:576:1PE:H141	2.47	0.50
7:D:577:1PE:H222	8:D:608:HOH:O	2.12	0.50
1:C:175:TYR:CD2	1:C:186[B]:MET:HG2	2.47	0.49
1:D:161:LYS:O	1:D:162:ASP:HB3	2.12	0.49
1:D:135[B]:MET:HG2	1:D:215[B]:MET:HE3	1.93	0.49
1:D:218:LEU:HD23	1:D:218:LEU:C	2.32	0.49
1:D:169:SER:HB3	1:D:190:LYS:HG2	1.95	0.49
1:D:247[B]:MET:HG3	1:D:272:PHE:CD1	2.47	0.49
1:B:207:LYS:O	1:B:238:VAL:HG11	2.12	0.49
1:B:253:SER:O	1:B:254:THR:C	2.50	0.48
1:D:203:ASP:OD2	3:D:571:EPE:H71	2.12	0.48
1:D:122:PHE:HE2	1:D:247[B]:MET:CE	2.26	0.48
1:C:170:THR:HG21	1:C:187:SER:HB2	1.94	0.48
1:A:188:LEU:HD21	1:A:193[B]:MET:CE	2.43	0.48
5:A:574:2PE:H122	1:B:112:PRO:HA	1.94	0.48
1:A:135[A]:MET:HG2	1:A:215[A]:MET:CE	2.43	0.48
1:A:252:LEU:HD23	1:A:264:ILE:HD13	1.94	0.48
1:B:182:ARG:HH12	1:C:130:GLU:CD	2.17	0.48
1:A:115:LEU:HD13	1:A:143:PRO:HB2	1.95	0.48
1:A:18:THR:HG22	6:B:575:PG4:H61	1.96	0.48
1:A:218:LEU:HD23	1:A:218:LEU:C	2.33	0.48
1:C:242:LEU:HD23	1:C:246:TYR:CD2	2.49	0.48
1:C:247[B]:MET:HG3	1:C:272:PHE:CE1	2.48	0.47
1:D:190:LYS:HA	1:D:190:LYS:HE2	1.95	0.47
1:B:120:LYS:HE3	8:B:691:HOH:O	2.15	0.47
1:C:186[B]:MET:HE1	1:C:215[B]:MET:CG	2.45	0.47
1:C:206[B]:MET:HE2	1:C:238:VAL:HG21	1.97	0.47
1:B:125:VAL:HG21	1:B:247[A]:MET:HE2	1.97	0.47
1:C:104:TYR:CZ	1:C:106:THR:HB	2.50	0.47
1:B:97:ILE:CG2	1:B:255:ILE:HD11	2.42	0.47
1:B:181:ASN:C	1:B:181:ASN:ND2	2.68	0.47
1:D:135[B]:MET:CE	1:D:219:LEU:HD21	2.45	0.47
1:A:157:VAL:HG11	1:A:193[B]:MET:HE2	1.97	0.47
5:A:574:2PE:H81	1:B:146:TYR:HB2	1.96	0.47
1:C:89:GLN:NE2	8:C:643:HOH:O	2.47	0.47
4:D:573:P6G:H142	8:D:600:HOH:O	2.14	0.47
1:D:256:ASN:HA	1:D:257:MET:HE3	1.96	0.47
1:A:115:LEU:CD1	1:A:143:PRO:HB2	2.44	0.47
1:A:203:ASP:OD2	3:A:570:EPE:H81	2.15	0.47
1:C:206[B]:MET:SD	1:C:242:LEU:HD22	2.54	0.47
1:D:125:VAL:HG21	1:D:247[A]:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247[B]:MET:CE	1:D:249:LEU:HD23	2.44	0.47
1:D:65:ALA:C	1:D:67:GLY:H	2.16	0.47
1:A:104:TYR:CZ	1:A:106:THR:HB	2.51	0.47
1:D:30:SER:HB2	1:D:37:LYS:HD3	1.97	0.47
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.80	0.46
1:A:218:LEU:O	1:A:218:LEU:HD23	2.15	0.46
1:A:143:PRO:HB3	1:B:146:TYR:CE1	2.51	0.46
1:D:138:ALA:HA	1:D:139:THR:HA	1.69	0.46
1:A:130:GLU:O	1:A:198:ASN:CB	2.63	0.46
1:B:207:LYS:O	1:B:238:VAL:CG1	2.63	0.46
1:A:97:ILE:CD1	1:A:97:ILE:O	2.64	0.46
1:D:190:LYS:CE	1:D:190:LYS:N	2.79	0.46
1:B:262:ILE:O	1:B:262:ILE:HG23	2.16	0.46
1:C:172:SER:C	1:C:173:ILE:HD12	2.35	0.46
1:B:234:GLU:O	1:B:234:GLU:HG3	2.16	0.46
1:C:108:ILE:HG23	1:C:114:VAL:HG11	1.98	0.46
1:C:173:ILE:HD13	1:C:218:LEU:CD1	2.45	0.46
1:C:247[B]:MET:CE	1:C:249:LEU:HD23	2.46	0.46
1:B:17:LEU:O	6:B:575:PG4:H42	2.16	0.46
1:B:206[B]:MET:HE1	1:B:246:TYR:CE1	2.51	0.46
1:A:123:ALA:HB1	1:A:152:LEU:HD13	1.97	0.46
1:D:206[B]:MET:HE3	1:D:238:VAL:CG1	2.46	0.46
1:B:62:VAL:O	1:B:67:GLY:HA3	2.16	0.46
1:A:133:VAL:CG1	1:A:199:VAL:HG22	2.46	0.46
1:B:138:ALA:HA	1:B:139:THR:HA	1.57	0.46
1:A:139:THR:HG21	1:B:160:ARG:NH2	2.31	0.46
1:D:247[B]:MET:HE1	1:D:249:LEU:CD2	2.46	0.46
1:A:59:LEU:HD22	1:A:69:VAL:HG22	1.98	0.46
1:D:259:GLU:OE1	1:D:260:LYS:N	2.49	0.45
1:C:153:ASN:HA	8:C:762:HOH:O	2.15	0.45
1:A:151:TYR:CZ	5:A:574:2PE:H211	2.52	0.45
1:D:91:LEU:HD21	1:D:108:ILE:HD13	1.98	0.45
1:B:255:ILE:HG12	1:B:256:ASN:N	2.31	0.45
1:C:242:LEU:HD12	1:C:242:LEU:HA	1.83	0.45
1:B:4:ARG:HG2	1:B:4:ARG:NH1	2.31	0.45
1:A:118:VAL:HG11	1:A:144:LEU:HD22	1.99	0.45
1:D:96:ARG:HB3	1:D:104:TYR:H	1.82	0.45
1:A:253:SER:O	1:A:254:THR:C	2.55	0.45
1:A:217:ASN:O	1:A:220:ASP:HB2	2.16	0.45
1:D:170:THR:HA	1:D:190:LYS:HD2	1.99	0.45
1:C:182:ARG:NH2	8:C:715:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LEU:HA	1:D:270:LEU:HD12	1.72	0.45
1:A:98:LEU:HB2	1:A:102:TYR:C	2.37	0.45
1:C:171:VAL:HG11	1:C:221:GLU:HB2	1.98	0.45
1:D:97:ILE:O	1:D:98:LEU:HD12	2.17	0.45
1:A:87:LEU:HD11	1:A:108:ILE:HD12	1.99	0.45
1:A:177:SER:OG	1:A:178:GLY:N	2.50	0.45
1:A:94:PRO:O	1:A:97:ILE:HG23	2.16	0.45
1:C:62:VAL:O	1:C:67:GLY:HA3	2.17	0.45
1:C:176:VAL:O	1:C:210:GLY:HA3	2.17	0.45
1:C:111:LYS:HE3	1:C:114:VAL:HG23	1.99	0.44
1:A:118:VAL:HG11	1:A:144:LEU:CD2	2.47	0.44
1:D:97:ILE:CG2	1:D:255:ILE:HD11	2.46	0.44
1:C:206[A]:MET:HE2	1:C:212:ILE:HD12	1.98	0.44
1:A:93:ASN:ND2	1:A:94:PRO:HD2	2.27	0.44
1:B:238:VAL:C	1:B:240:GLU:N	2.69	0.44
1:C:77:GLN:HE21	1:C:274:LYS:HG3	1.82	0.44
1:D:154:VAL:HB	1:D:155:PRO:HD2	1.99	0.44
1:A:18:THR:HG22	6:B:575:PG4:C6	2.47	0.44
1:C:238:VAL:C	1:C:240:GLU:H	2.21	0.44
1:B:122:PHE:HD2	1:B:247[A]:MET:HE3	1.82	0.44
1:D:171:VAL:N	1:D:190:LYS:HD3	2.32	0.44
1:C:2:LYS:HG2	1:C:34:GLU:HB2	1.98	0.44
1:A:256:ASN:HA	1:A:257:MET:HE1	2.00	0.44
1:A:256:ASN:HB3	1:A:259:GLU:HB3	1.98	0.44
1:A:23:LEU:HD22	4:A:572:P6G:H91	1.99	0.44
1:C:135[B]:MET:HE3	1:C:215[B]:MET:HB3	2.00	0.44
1:D:171:VAL:H	1:D:190:LYS:CE	2.31	0.44
1:D:206[B]:MET:HE3	1:D:238:VAL:HG13	2.00	0.44
1:C:254:THR:HA	8:C:741:HOH:O	2.18	0.44
1:D:122:PHE:HE2	1:D:247[B]:MET:HE2	1.82	0.44
1:B:157:VAL:HG21	1:B:193[A]:MET:HE2	2.00	0.44
1:C:93:ASN:ND2	1:C:94:PRO:HD2	2.28	0.44
1:A:173:ILE:HG22	1:A:174:ASN:N	2.32	0.44
1:D:171:VAL:HG11	1:D:221:GLU:HB2	2.00	0.44
1:B:170:THR:HG22	1:B:171:VAL:N	2.32	0.44
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.82	0.44
1:D:24:ILE:HA	1:D:25:PRO:HD3	1.87	0.44
7:C:576:1PE:H121	1:D:146:TYR:HB3	1.98	0.43
1:A:138:ALA:HA	1:A:139:THR:HA	1.63	0.43
7:C:576:1PE:H142	7:D:577:1PE:H131	2.00	0.43
1:C:270:LEU:HA	1:C:270:LEU:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:SER:O	1:C:45:THR:HG23	2.18	0.43
1:D:87:LEU:HD21	1:D:232:LEU:HD11	2.00	0.43
1:C:180:SER:C	1:C:182:ARG:N	2.70	0.43
1:B:171:VAL:HG11	1:B:221:GLU:CB	2.49	0.43
1:A:135[B]:MET:HE2	1:A:215[B]:MET:SD	2.58	0.43
1:D:253:SER:HB2	1:D:263:GLU:HB2	2.00	0.43
1:C:2:LYS:HZ2	1:C:2:LYS:HB3	1.80	0.43
1:D:8:ARG:O	1:D:12:LEU:HB2	2.19	0.43
1:D:190:LYS:CD	1:D:190:LYS:N	2.82	0.43
1:B:171:VAL:HG23	1:B:190:LYS:HG2	2.01	0.43
1:B:135[B]:MET:HE1	1:B:219:LEU:HD21	2.01	0.43
1:B:177:SER:OG	1:B:184:GLN:NE2	2.48	0.43
1:D:274:LYS:C	1:D:276:ASN:N	2.71	0.43
1:C:107:ASP:OD2	1:C:108:ILE:HD12	2.18	0.43
1:B:142:ILE:N	1:B:143:PRO:HD2	2.34	0.43
1:D:238:VAL:HA	1:D:241:ARG:CZ	2.49	0.42
1:D:8:ARG:HG3	1:D:33:TYR:CG	2.54	0.42
1:A:257:MET:SD	1:A:257:MET:N	2.92	0.42
1:C:241:ARG:HG3	1:C:241:ARG:HH11	1.85	0.42
1:D:171:VAL:HG23	1:D:190:LYS:CD	2.50	0.42
1:C:1:MET:HG2	1:C:2:LYS:N	2.33	0.42
1:C:138:ALA:HA	1:C:139:THR:HA	1.64	0.42
1:B:153:ASN:HA	8:B:721:HOH:O	2.20	0.42
1:A:180:SER:OG	1:A:182:ARG:HG2	2.20	0.42
1:C:122:PHE:CE2	1:C:247[B]:MET:HE1	2.55	0.42
1:A:252:LEU:O	1:A:252:LEU:HD13	2.20	0.42
1:C:159:VAL:HG11	1:C:186[B]:MET:HE3	2.01	0.42
1:D:204:ASP:O	1:D:232:LEU:HB3	2.20	0.42
1:B:37:LYS:HG2	8:B:604:HOH:O	2.18	0.42
5:A:574:2PE:H271	6:B:575:PG4:H62	2.01	0.42
1:D:26:LEU:HD23	8:D:681:HOH:O	2.20	0.42
1:C:24:ILE:HA	1:C:25:PRO:HD3	1.95	0.42
1:A:97:ILE:C	1:A:98:LEU:HD12	2.40	0.41
1:B:93:ASN:ND2	1:B:95:GLU:HB2	2.35	0.41
1:D:132:ASP:HB2	1:D:197:SER:HB2	2.02	0.41
1:A:231:VAL:O	1:A:248:SER:HA	2.20	0.41
1:A:170:THR:CG2	1:A:187:SER:HB2	2.50	0.41
1:C:272:PHE:N	1:C:272:PHE:CD1	2.88	0.41
1:D:171:VAL:N	1:D:190:LYS:CD	2.83	0.41
1:B:206[A]:MET:HE1	1:B:212:ILE:HD12	2.02	0.41
1:A:131:ILE:HD13	1:A:200:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135[B]:MET:SD	1:A:219:LEU:HD11	2.61	0.41
1:C:133:VAL:CG1	1:C:199:VAL:HG22	2.50	0.41
1:A:18:THR:CG2	6:B:575:PG4:H61	2.50	0.41
1:D:206[A]:MET:HE3	1:D:212:ILE:CD1	2.51	0.41
1:B:238:VAL:C	1:B:240:GLU:H	2.24	0.41
1:C:234:GLU:HG3	1:C:234:GLU:O	2.19	0.41
1:D:115:LEU:HD13	1:D:143:PRO:HB2	2.02	0.41
1:A:160:ARG:HE	1:A:160:ARG:HA	1.85	0.41
1:B:182:ARG:NH1	1:C:130:GLU:CD	2.74	0.41
1:C:171:VAL:HG11	1:C:221:GLU:CB	2.51	0.41
1:D:238:VAL:HA	1:D:241:ARG:NE	2.36	0.41
1:A:108:ILE:HG13	1:A:109:LEU:N	2.36	0.41
1:B:122:PHE:HD2	1:B:247[A]:MET:CE	2.34	0.41
1:C:262:ILE:O	1:C:262:ILE:HG23	2.21	0.41
1:B:16:LEU:HD13	1:B:59:LEU:HD11	2.03	0.41
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.75	0.40
1:C:206[A]:MET:HE2	1:C:212:ILE:CD1	2.51	0.40
1:C:180:SER:O	1:C:182:ARG:N	2.54	0.40
1:A:204:ASP:O	1:A:232:LEU:HB3	2.21	0.40
1:D:121:LEU:O	1:D:121:LEU:HD23	2.22	0.40
1:D:190:LYS:NZ	1:D:222:PHE:CZ	2.75	0.40
1:C:256:ASN:HD22	1:C:259:GLU:CB	2.31	0.40
1:B:135[A]:MET:HE3	1:B:219:LEU:HD21	2.03	0.40
1:A:130:GLU:O	1:A:198:ASN:HB3	2.20	0.40
1:D:102:TYR:N	1:D:102:TYR:CD1	2.89	0.40
1:C:135[B]:MET:CE	1:C:215[B]:MET:HB3	2.52	0.40
1:D:255:ILE:O	1:D:255:ILE:HG23	2.22	0.40
1:A:60:LEU:CD2	4:A:572:P6G:H62	2.52	0.40
1:A:171:VAL:HG12	1:A:172:SER:N	2.36	0.40
1:A:195:THR:HB	1:A:222:PHE:O	2.21	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	274/291 (94%)	258 (94%)	13 (5%)	3 (1%)	17	14
1	B	273/291 (94%)	262 (96%)	8 (3%)	3 (1%)	17	14
1	C	274/291 (94%)	265 (97%)	7 (3%)	2 (1%)	26	25
1	D	273/291 (94%)	258 (94%)	12 (4%)	3 (1%)	17	14
All	All	1094/1164 (94%)	1043 (95%)	40 (4%)	11 (1%)	19	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	THR
1	B	179	SER
1	B	254	THR
1	D	254	THR
1	B	169	SER
1	C	181	ASN
1	D	221	GLU
1	D	260	LYS
1	A	177	SER
1	A	221	GLU
1	C	239	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/250 (95%)	227 (95%)	11 (5%)	33	40
1	B	237/250 (95%)	222 (94%)	15 (6%)	22	24
1	C	238/250 (95%)	225 (94%)	13 (6%)	27	30
1	D	237/250 (95%)	226 (95%)	11 (5%)	33	40
All	All	950/1000 (95%)	900 (95%)	50 (5%)	29	32



All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	93	ASN
1	A	130	GLU
1	A	139	THR
1	A	140	LYS
1	A	152	LEU
1	A	160	ARG
1	A	162	ASP
1	A	257	MET
1	A	270	LEU
1	A	274	LYS
1	B	2	LYS
1	B	3	PHE
1	B	23	LEU
1	B	98	LEU
1	B	116	SER
1	B	152	LEU
1	B	173	ILE
1	B	176	VAL
1	B	181	ASN
1	B	182	ARG
1	B	191	ARG
1	B	242	LEU
1	B	244	ASP
1	B	259	GLU
1	B	270	LEU
1	C	3	PHE
1	C	23	LEU
1	C	59	LEU
1	C	82	GLU
1	C	93	ASN
1	C	98	LEU
1	C	130	GLU
1	C	152	LEU
1	C	182	ARG
1	C	259	GLU
1	C	265[A]	GLN
1	C	265[B]	GLN
1	C	270	LEU
1	D	6[A]	SER
1	D	6[B]	SER
1	D	61	THR

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Mol	Chain	Res	Type
1	D	112	PRO
1	D	152	LEU
1	D	190	LYS
1	D	257	MET
1	D	258	LYS
1	D	259	GLU
1	D	270	LEU
1	D	274	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	53	GLN
1	A	89	GLN
1	A	93	ASN
1	A	153	ASN
1	A	184	GLN
1	A	213	ASN
1	A	223	ASN
1	A	265	GLN
1	A	266	ASN
1	B	54	GLN
1	B	89	GLN
1	B	153	ASN
1	B	181	ASN
1	B	184	GLN
1	B	223	ASN
1	B	266	ASN
1	C	54	GLN
1	C	77	GLN
1	C	89	GLN
1	C	93	ASN
1	C	153	ASN
1	C	256	ASN
1	C	266	ASN
1	D	77	GLN
1	D	89	GLN
1	D	184	GLN
1	D	213	ASN
1	D	223	ASN
1	D	266	ASN

### 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 ⓘ

16 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	$\# Z  > 2$
3	EPE	A	570	-	14,15,15	1.08	0	18,20,20	0.80	0
4	P6G	A	572	-	18,18,18	0.46	0	17,17,17	0.33	0
5	2PE	A	574	-	27,27,27	0.52	0	26,26,26	0.30	0
2	SO4	A	581	-	4,4,4	0.10	0	6,6,6	0.39	0
6	PG4	B	575	-	12,12,12	0.39	0	11,11,11	0.49	0
2	SO4	B	582	-	4,4,4	0.11	0	6,6,6	0.25	0
2	SO4	B	586	-	4,4,4	0.30	0	6,6,6	0.16	0
2	SO4	B	589	-	4,4,4	0.28	0	6,6,6	0.17	0
7	1PE	C	576	-	15,15,15	0.40	0	14,14,14	0.45	0
2	SO4	C	583	-	4,4,4	0.23	0	6,6,6	0.27	0
2	SO4	C	587	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	C	590	-	4,4,4	0.28	0	6,6,6	0.07	0
3	EPE	D	571	-	14,15,15	1.10	0	18,20,20	0.83	0
4	P6G	D	573	-	18,18,18	0.48	0	17,17,17	0.37	0
7	1PE	D	577	-	15,15,15	0.59	0	14,14,14	0.36	0
2	SO4	D	584	-	4,4,4	0.19	0	6,6,6	0.43	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
3	EPE	A	570	-	-	0/9/19/19	0/1/1/1
4	P6G	A	572	-	-	0/16/16/16	0/0/0/0
5	2PE	A	574	-	-	0/25/25/25	0/0/0/0
2	SO4	A	581	-	-	0/0/0/0	0/0/0/0
6	PG4	B	575	-	-	0/10/10/10	0/0/0/0
2	SO4	B	582	-	-	0/0/0/0	0/0/0/0
2	SO4	B	586	-	-	0/0/0/0	0/0/0/0
2	SO4	B	589	-	-	0/0/0/0	0/0/0/0
7	1PE	C	576	-	-	0/13/13/13	0/0/0/0
2	SO4	C	583	-	-	0/0/0/0	0/0/0/0
2	SO4	C	587	-	-	0/0/0/0	0/0/0/0
2	SO4	C	590	-	-	0/0/0/0	0/0/0/0
3	EPE	D	571	-	-	0/9/19/19	0/1/1/1
4	P6G	D	573	-	-	0/16/16/16	0/0/0/0
7	1PE	D	577	-	-	0/13/13/13	0/0/0/0
2	SO4	D	584	-	-	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.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	570	EPE	3	0
4	A	572	P6G	2	0
5	A	574	2PE	10	0
6	B	575	PG4	6	0
7	C	576	1PE	5	0
3	D	571	EPE	1	0
4	D	573	P6G	2	0
7	D	577	1PE	4	0

## 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	270/291 (92%)	0.68	44 (16%) 2 2	23, 46, 108, 163	0
1	B	269/291 (92%)	0.44	36 (13%) 4 4	23, 43, 94, 125	0
1	C	269/291 (92%)	0.33	29 (10%) 8 7	22, 39, 88, 115	0
1	D	270/291 (92%)	0.61	41 (15%) 3 3	24, 46, 97, 154	0
All	All	1078/1164 (92%)	0.51	150 (13%) 4 3	22, 43, 99, 163	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	11.6
1	B	179	SER	11.1
1	A	257	MET	10.6
1	D	257	MET	8.6
1	A	275	ASP	7.8
1	A	256	ASN	7.7
1	D	275	ASP	7.5
1	D	258	LYS	7.1
1	C	180	SER	6.7
1	A	258	LYS	6.5
1	C	179	SER	6.0
1	D	183	ILE	5.9
1	B	238	VAL	5.8
1	C	241	ARG	5.5
1	C	168	GLY	5.4
1	A	182	ARG	5.4
1	C	169	SER	5.4
1	A	101	GLY	5.3
1	D	181	ASN	5.3
1	A	180	SER	5.2
1	D	256	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	64	GLY	5.1
1	A	183	ILE	5.1
1	A	276	ASN	5.0
1	A	185	THR	5.0
1	A	181	ASN	4.9
1	B	254	THR	4.9
1	A	260	LYS	4.9
1	D	169	SER	4.8
1	D	276	ASN	4.7
1	A	179	SER	4.7
1	C	274	LYS	4.7
1	A	168	GLY	4.6
1	A	100	GLY	4.5
1	A	176	VAL	4.4
1	D	182	ARG	4.4
1	A	193[A]	MET	4.3
1	D	66	ALA	4.2
1	D	259	GLU	4.2
1	A	259	GLU	4.1
1	D	162	ASP	4.1
1	D	255	ILE	4.1
1	C	258	LYS	4.1
1	B	180	SER	4.1
1	B	1	MET	4.0
1	A	169	SER	3.9
1	B	258	LYS	3.9
1	C	206[A]	MET	3.8
1	C	247[A]	MET	3.8
1	D	179	SER	3.8
1	D	206[A]	MET	3.8
1	D	185	THR	3.8
1	B	206[A]	MET	3.8
1	A	261	SER	3.7
1	C	178	GLY	3.7
1	A	162	ASP	3.7
1	D	247[A]	MET	3.6
1	D	180	SER	3.6
1	A	254	THR	3.6
1	B	168	GLY	3.6
1	B	169	SER	3.6
1	C	238	VAL	3.5
1	B	239	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	260	LYS	3.5
1	A	274	LYS	3.4
1	B	178	GLY	3.4
1	D	97	ILE	3.4
1	D	168	GLY	3.3
1	A	63	PRO	3.3
1	D	274	LYS	3.3
1	A	171	VAL	3.3
1	C	237	GLY	3.3
1	A	215[A]	MET	3.2
1	D	65	ALA	3.2
1	A	97	ILE	3.1
1	B	237	GLY	3.1
1	C	215[A]	MET	3.1
1	C	135[A]	MET	3.1
1	A	192	SER	3.0
1	C	239	ASP	3.0
1	B	241	ARG	3.0
1	B	255	ILE	3.0
1	B	195	THR	3.0
1	B	102	TYR	2.9
1	C	254	THR	2.9
1	A	247[A]	MET	2.9
1	D	193[A]	MET	2.9
1	A	206[A]	MET	2.9
1	B	247[A]	MET	2.8
1	C	193[A]	MET	2.8
1	A	241	ARG	2.8
1	B	135[A]	MET	2.8
1	C	243	VAL	2.8
1	A	135[A]	MET	2.8
1	B	97	ILE	2.7
1	D	135[A]	MET	2.7
1	B	170	THR	2.7
1	D	62	VAL	2.7
1	C	202	ILE	2.7
1	A	102	TYR	2.7
1	B	240	GLU	2.7
1	A	190	LYS	2.7
1	B	261	SER	2.6
1	A	184	GLN	2.6
1	A	99	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	171	VAL	2.6
1	D	3	PHE	2.6
1	A	2	LYS	2.6
1	D	100	GLY	2.6
1	B	257	MET	2.6
1	D	161	LYS	2.5
1	D	99	PRO	2.5
1	B	259	GLU	2.5
1	D	190	LYS	2.5
1	C	201	ILE	2.5
1	A	93	ASN	2.5
1	C	257[A]	MET	2.5
1	B	162	ASP	2.5
1	C	162	ASP	2.5
1	A	174	ASN	2.5
1	A	195	THR	2.4
1	D	2	LYS	2.4
1	B	182	ARG	2.4
1	C	229	ILE	2.4
1	D	63	PRO	2.4
1	D	195	THR	2.4
1	A	161	LYS	2.4
1	B	215[A]	MET	2.3
1	B	89	GLN	2.3
1	C	194	LYS	2.3
1	B	262	ILE	2.3
1	C	230	GLY	2.3
1	D	170	THR	2.3
1	B	274	LYS	2.3
1	B	181	ASN	2.2
1	B	193[A]	MET	2.2
1	B	85	GLN	2.2
1	B	231	VAL	2.2
1	A	4	ARG	2.2
1	B	256	ASN	2.2
1	D	215[A]	MET	2.2
1	C	231	VAL	2.1
1	A	186[A]	MET	2.1
1	C	240	GLU	2.1
1	D	172	SER	2.1
1	D	221	GLU	2.1
1	B	194	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	186[A]	MET	2.1
1	C	1	MET	2.0
1	C	261	SER	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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	589	5/5	0.72	0.28	9.14	84,84,92,92	5
2	SO4	C	590	5/5	0.77	0.32	6.07	88,88,91,92	5
6	PG4	B	575	13/13	0.85	0.35	5.26	75,83,94,98	0
4	P6G	A	572	19/19	0.85	0.25	5.08	48,81,91,92	0
7	1PE	D	577	16/16	0.78	0.35	4.85	80,94,103,107	0
5	2PE	A	574	28/28	0.80	0.30	4.67	79,91,100,102	0
3	EPE	A	570	15/15	0.74	0.50	4.00	93,106,109,110	15
3	EPE	D	571	15/15	0.76	0.53	3.80	100,104,112,115	15
7	1PE	C	576	16/16	0.79	0.28	3.30	82,93,96,98	0
4	P6G	D	573	19/19	0.83	0.24	2.11	53,77,97,98	0
2	SO4	C	583	5/5	0.99	0.14	-0.77	42,44,54,69	0
2	SO4	B	582	5/5	0.99	0.10	-1.03	50,51,64,66	0
2	SO4	A	581	5/5	0.98	0.11	-1.06	56,56,67,68	0
2	SO4	C	587	5/5	0.97	0.10	-1.29	55,55,59,63	5
2	SO4	D	584	5/5	0.97	0.10	-1.32	52,53,57,64	0
2	SO4	B	586	5/5	0.95	0.11	-	56,62,65,67	5

## 6.5 Other polymers

There are no such residues in this entry.