



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:10 AM EST

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

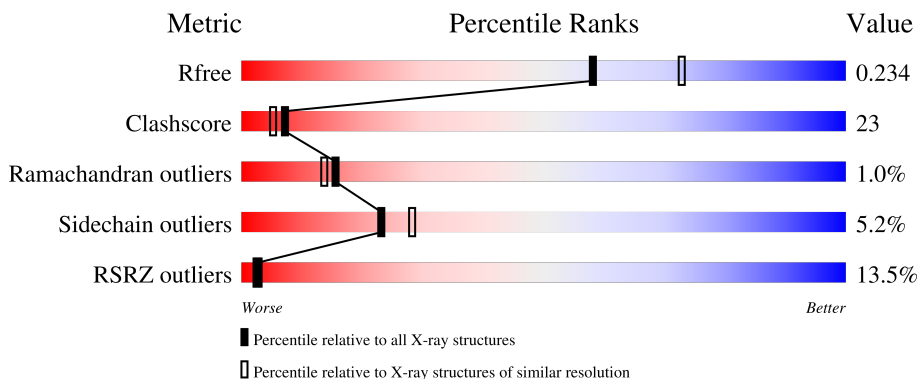
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 of 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	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	A	570	-	-	-	X
3	EPE	D	571	-	-	-	X

## 2 Entry composition i

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

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).



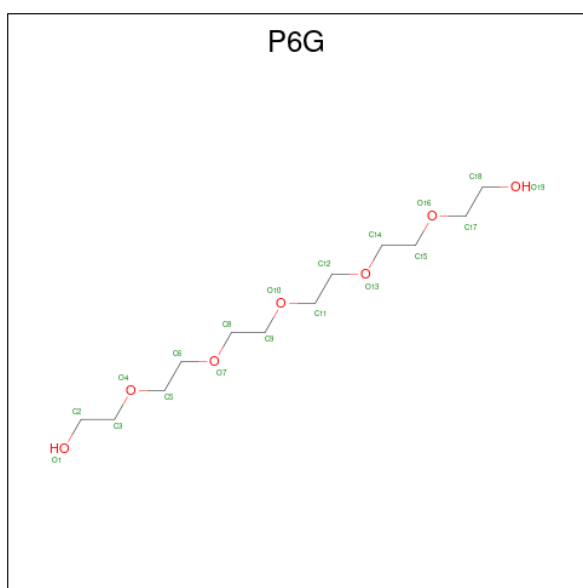
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- 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).



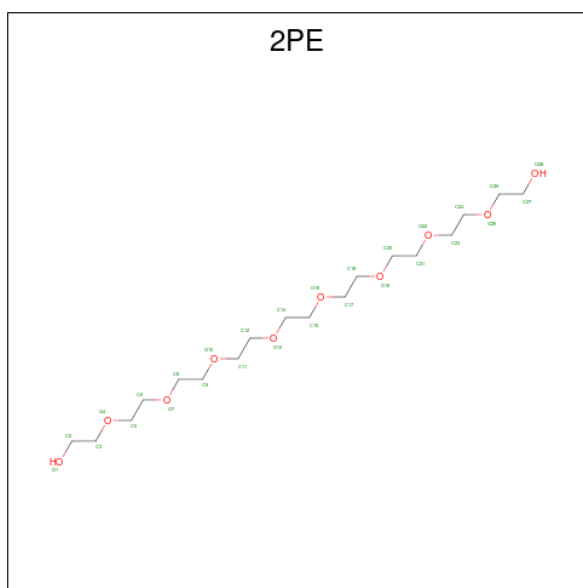
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	15	8	2	4	1	0	0
3	D	1	15	8	2	4	1	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



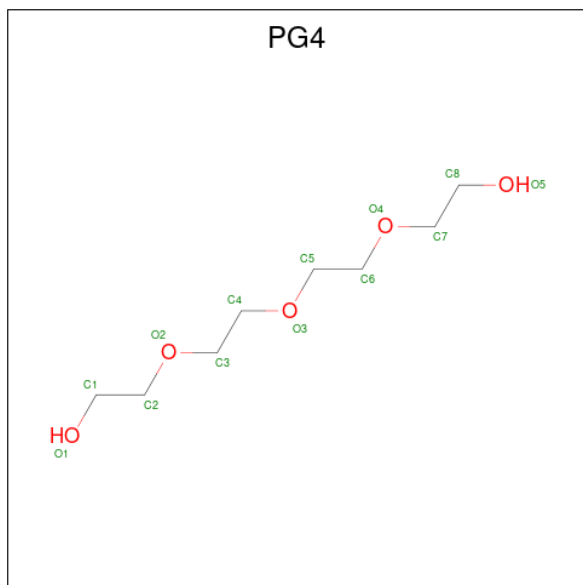
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	19	12	7	0	0
4	D	1	19	12	7	0	0

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula:  $C_{18}H_{38}O_{10}$ ).



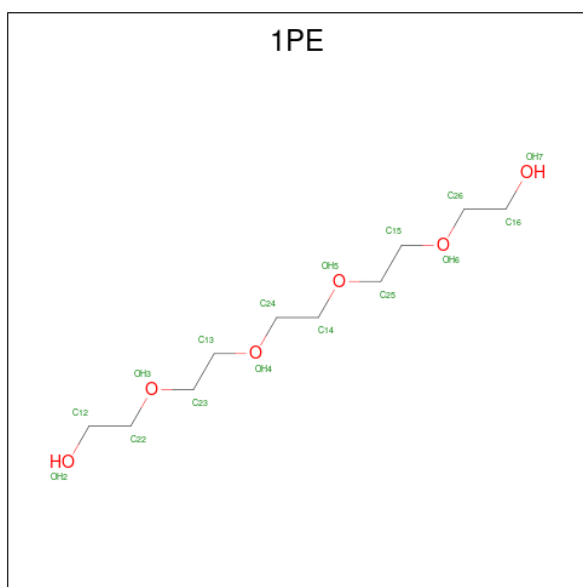
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	A	1	Total	C	O	0	0
			28	18	10		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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:  $C_{10}H_{22}O_6$ ).



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.

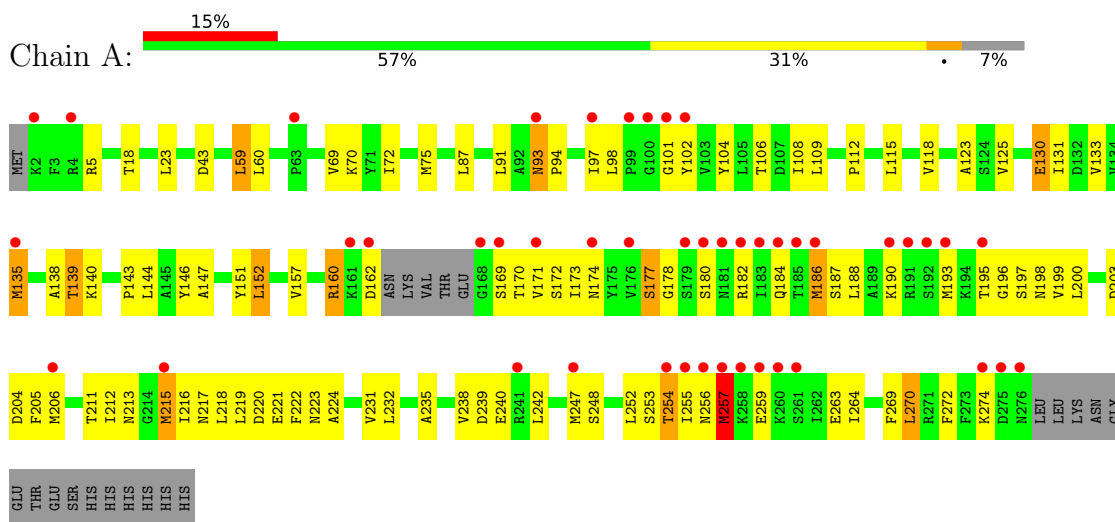
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	121	Total	O	0	0
			121	121		
8	B	138	Total	O	0	0
			138	138		
8	C	177	Total	O	0	0
			177	177		
8	D	132	Total	O	0	0
			132	132		



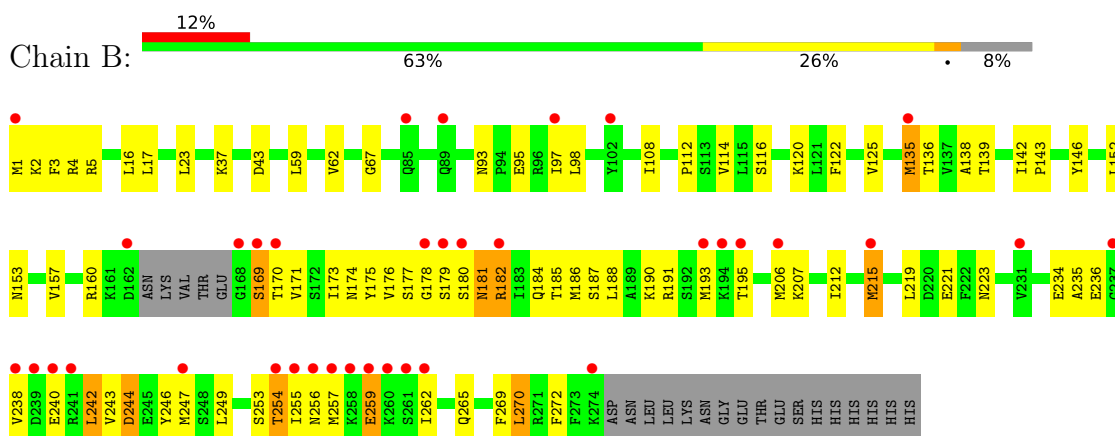
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

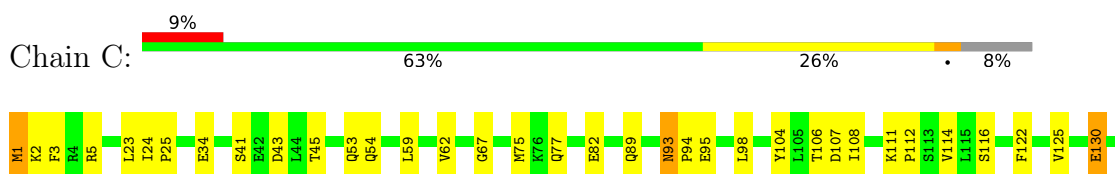
#### • Molecule 1: PUR OPERON REPRESSOR

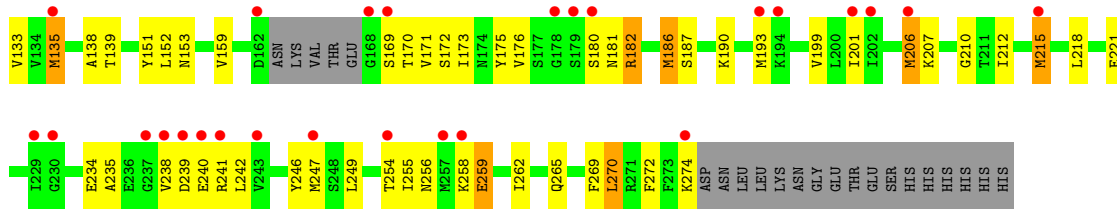


#### • Molecule 1: PUR OPERON REPRESSOR

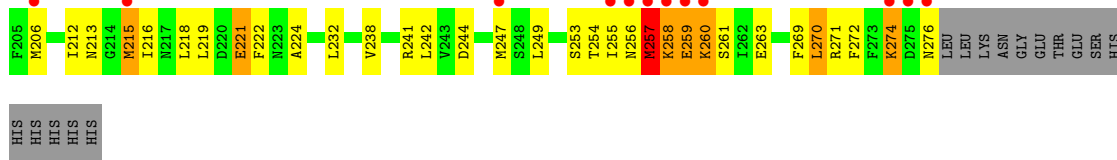
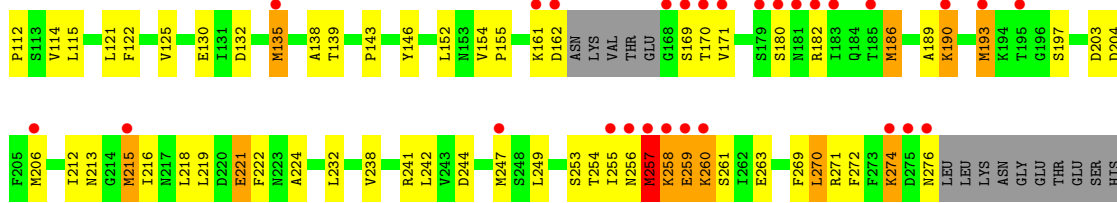
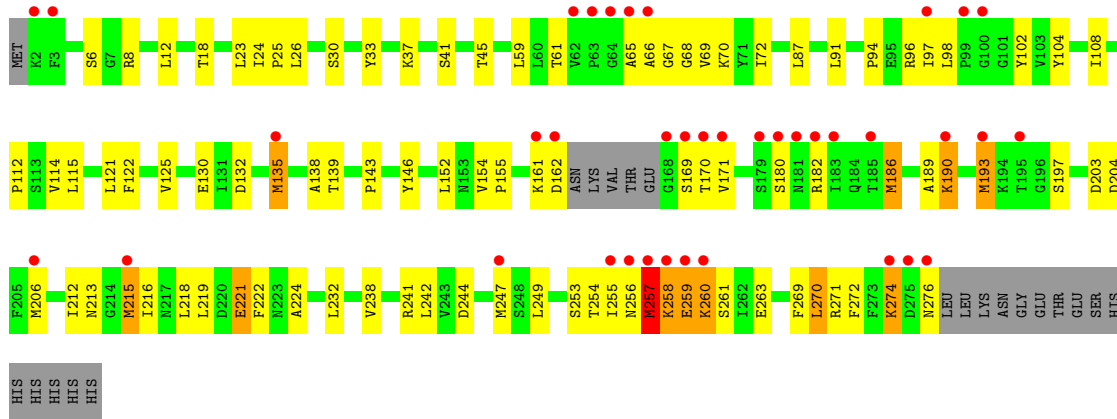


#### • Molecule 1: PUR OPERON REPRESSOR





● 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) 93.2 (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)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.188 , 0.237 0.186 , 0.234	Depositor DCC
$R_{free}$ test set	3335 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 2PE, EPE, PG4, 1PE, SO4, P6G

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:NZ	1:D:190:LYS:HA	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:HH11	1:B:182:ARG:CG	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:C:135[A]:MET:CG	1:C:215[A]:MET:HE3	2.26	0.64
1:D:190:LYS:CE	1:D:190:LYS:CA	2.75	0.64
1:C:256:ASN:ND2	1:C:259:GLU:CD	2.49	0.64
1:D:23:LEU:HB2	4:D:573:P6G:H122	1.80	0.63
1:D:171:VAL:HB	1:D:190:LYS:HE3	1.81	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: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:D:169:SER:O	1:D:190:LYS:HD2	1.99	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:93:ASN:HD22	1:A:94:PRO:CD	2.13	0.62
1:A:98:LEU:HB2	1:A:102:TYR:O	2.00	0.62
1:A:219:LEU:HB3	1:A:224:ALA:HB3	1.80	0.62
1:B:247[B]:MET:HE1	1:B:249:LEU:HD23	1.82	0.62
1:C:93:ASN:HD22	1:C:93:ASN:C	2.02	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:C:180:SER:C	1:C:182:ARG:H	2.04	0.60
1:D:169:SER:HB2	1:D:190:LYS:HB2	1.84	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:B:195:THR:HG23	1:B:223:ASN:HB2	1.83	0.59
1:B:247[B]:MET:HG3	1:B:272:PHE:CD1	2.37	0.59
1:C:256:ASN:ND2	1:C:259:GLU:H	2.00	0.59
1:B:206[A]:MET:CE	1:B:212:ILE:HD12	2.32	0.59
1:C:170:THR:CG2	1:C:187:SER:HB2	2.31	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:93:ASN:ND2	1:C:95:GLU:H	2.00	0.59
1:C:173:ILE:HD13	1:C:218:LEU:HD13	1.85	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:A:139:THR:HG21	1:B:160:ARG:HH22	1.68	0.58
1:B:174:ASN:OD1	1:B:185:THR:HG22	2.03	0.58
1:D:257:MET:HB3	8:D:705:HOH:O	2.02	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:HG21	1:B:187:SER:HB2	1.84	0.58
1:B:170:THR:CG2	1:B:187:SER:HB2	2.33	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:H251	7:D:577:1PE:H122	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: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:D:189:ALA:C	1:D:190:LYS:HE2	2.25	0.56
1:A:213:ASN:ND2	1:A:242:LEU:HD12	2.21	0.56
1:A:239:ASP:O	1:A:240:GLU:HG3	2.06	0.55
1:D:259:GLU:O	1:D:261:SER:N	2.39	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:169:SER:O	1:C:190:LYS:HB2	2.07	0.54
1:C:201:ILE:HG23	1:C:215[A]:MET:HE1	1.88	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
5:A:574:2PE:H172	5:A:574:2PE:H112	1.88	0.54
1:C:256:ASN:ND2	1:C:259:GLU:OE2	2.40	0.54
1:D:26:LEU:HD21	8:D:697:HOH:O	2.07	0.54
1:C:93:ASN:C	1:C:93:ASN:ND2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135[A]:MET:SD	1:C:215[A]:MET:HE3	2.48	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:B:235:ALA:O	1:B:238:VAL:HG13	2.08	0.53
1:D:190:LYS:HZ3	1:D:190:LYS:CA	2.20	0.53
1:A:190:LYS:O	1:A:190:LYS:HD3	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:A:5:ARG:NE	1:A:43:ASP:OD1	2.42	0.52
1:D:125:VAL:HG11	1:D:247[A]:MET:HE2	1.92	0.52
1:A:174:ASN:HA	1:A:184:GLN:O	2.09	0.52
1:B:5:ARG:HD3	1:B:43:ASP:OD1	2.10	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:A:256:ASN:HA	1:A:257:MET:HE3	1.92	0.51
1:C:173:ILE:HD11	1:C:221:GLU:HG3	1.92	0.51
1:D:190:LYS:CA	1:D:190:LYS:HE2	2.40	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:C:151:TYR:CZ	7:C:576:1PE:H141	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASN:HD22	1:D:242:LEU:CD1	2.24	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:C:170:THR:HG21	1:C:187:SER:HB2	1.94	0.48
1:D:122:PHE:HE2	1:D:247[B]:MET:CE	2.26	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:A:115:LEU:HD13	1:A:143:PRO:HB2	1.95	0.48
1:B:182:ARG:HH12	1:C:130:GLU:CD	2.17	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:B:120:LYS:HE3	8:B:691:HOH:O	2.15	0.47
1:D:190:LYS:HA	1:D:190:LYS:HE2	1.95	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: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: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: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
1:D:135[B]:MET:CE	1:D:219:LEU:HD21	2.45	0.47
1:D:256:ASN:HA	1:D:257:MET:HE3	1.96	0.47
4:D:573:P6G:H142	8:D:600:HOH:O	2.14	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:A:104:TYR:CZ	1:A:106:THR:HB	2.51	0.47
1:C:206[B]:MET:SD	1:C:242:LEU:HD22	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:SER:HB2	1:D:37:LYS:HD3	1.97	0.47
1:D:65:ALA:C	1:D:67:GLY:H	2.16	0.47
1:D:125:VAL:HG21	1:D:247[A]:MET:CE	2.45	0.47
1:D:247[B]:MET:CE	1:D:249:LEU:HD23	2.44	0.47
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.80	0.46
1:A:218:LEU:HD23	1:A:218:LEU:O	2.15	0.46
1:A:130:GLU:O	1:A:198:ASN:CB	2.63	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:B:207:LYS:O	1:B:238:VAL:CG1	2.63	0.46
1:A:97:ILE:O	1:A:97:ILE:CD1	2.64	0.46
1:B:262:ILE:HG23	1:B:262:ILE:O	2.16	0.46
1:D:190:LYS:CE	1:D:190:LYS:N	2.79	0.46
1:B:234:GLU:HG3	1:B:234:GLU:O	2.16	0.46
1:C:108:ILE:HG23	1:C:114:VAL:HG11	1.98	0.46
1:C:172:SER:C	1:C:173:ILE:HD12	2.35	0.46
1:A:123:ALA:HB1	1:A:152:LEU:HD13	1.97	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: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:A:133:VAL:CG1	1:A:199:VAL:HG22	2.46	0.46
1:B:62:VAL:O	1:B:67:GLY:HA3	2.16	0.46
1:D:206[B]:MET:HE3	1:D:238:VAL:CG1	2.46	0.46
1:A:139:THR:HG21	1:B:160:ARG:NH2	2.31	0.46
1:B:138:ALA:HA	1:B:139:THR:HA	1.57	0.46
1:A:59:LEU:HD22	1:A:69:VAL:HG22	1.98	0.46
1:D:247[B]:MET:HE1	1:D:249:LEU:CD2	2.46	0.46
1:C:153:ASN:HA	8:C:762:HOH:O	2.15	0.45
1:D:259:GLU:OE1	1:D:260:LYS:N	2.49	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:A:118:VAL:HG11	1:A:144:LEU:HD22	1.99	0.45
1:B:4:ARG:HG2	1:B:4:ARG:NH1	2.31	0.45
1:C:242:LEU:HD12	1:C:242:LEU:HA	1.83	0.45
1:D:96:ARG:HB3	1:D:104:TYR:H	1.82	0.45
1:A:217:ASN:O	1:A:220:ASP:HB2	2.16	0.45
1:A:253:SER:O	1:A:254:THR:C	2.55	0.45
1:C:182:ARG:NH2	8:C:715:HOH:O	2.50	0.45
1:D:170:THR:HA	1:D:190:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LEU:HD12	1:D:270:LEU:HA	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: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:D:97:ILE:O	1:D:98:LEU:HD12	2.17	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:A:118:VAL:HG11	1:A:144:LEU:CD2	2.47	0.44
1:C:111:LYS:HE3	1:C:114:VAL:HG23	1.99	0.44
1:C:206[A]:MET:HE2	1:C:212:ILE:HD12	1.98	0.44
1:D:97:ILE:CG2	1:D:255:ILE:HD11	2.46	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:B:122:PHE:HD2	1:B:247[A]:MET:HE3	1.82	0.44
1:C:238:VAL:C	1:C:240:GLU:H	2.21	0.44
1:A:23:LEU:HD22	4:A:572:P6G:H91	1.99	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:C:2:LYS:HG2	1:C:34:GLU:HB2	1.98	0.44
1:D:171:VAL:N	1:D:190:LYS:HD3	2.32	0.44
1:C:135[B]:MET:HE3	1:C:215[B]:MET:HB3	2.00	0.44
1:B:157:VAL:HG21	1:B:193[A]:MET:HE2	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: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:A:173:ILE:HG22	1:A:174:ASN:N	2.32	0.44
1:C:93:ASN:ND2	1:C:94:PRO:HD2	2.28	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
1:D:171:VAL:HG11	1:D:221:GLU:HB2	2.00	0.44
1:A:138:ALA:HA	1:A:139:THR:HA	1.63	0.43
7:C:576:1PE:H121	1:D:146:TYR:HB3	1.98	0.43
7:C:576:1PE:H142	7:D:577:1PE:H131	2.00	0.43
1:C:41:SER:O	1:C:45:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD12	1:C:270:LEU:HA	1.82	0.43
1:D:87:LEU:HD21	1:D:232:LEU:HD11	2.00	0.43
1:B:171:VAL:HG11	1:B:221:GLU:CB	2.49	0.43
1:C:180:SER:C	1:C:182:ARG:N	2.70	0.43
1:A:135[B]:MET:HE2	1:A:215[B]:MET:SD	2.58	0.43
1:C:2:LYS:HB3	1:C:2:LYS:HZ2	1.80	0.43
1:D:8:ARG:O	1:D:12:LEU:HB2	2.19	0.43
1:D:253:SER:HB2	1:D:263:GLU:HB2	2.00	0.43
1:B:135[B]:MET:HE1	1:B:219:LEU:HD21	2.01	0.43
1:B:142:ILE:N	1:B:143:PRO:HD2	2.34	0.43
1:B:171:VAL:HG23	1:B:190:LYS:HG2	2.01	0.43
1:B:177:SER:OG	1:B:184:GLN:NE2	2.48	0.43
1:C:107:ASP:OD2	1:C:108:ILE:HD12	2.18	0.43
1:D:190:LYS:N	1:D:190:LYS:CD	2.82	0.43
1:D:274:LYS:C	1:D:276:ASN:N	2.71	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:HH11	1:C:241:ARG:HG3	1.85	0.42
1:C:1:MET:HG2	1:C:2:LYS:N	2.33	0.42
1:D:171:VAL:HG23	1:D:190:LYS:CD	2.50	0.42
1:A:180:SER:OG	1:A:182:ARG:HG2	2.20	0.42
1:B:153:ASN:HA	8:B:721:HOH:O	2.20	0.42
1:C:138:ALA:HA	1:C:139:THR:HA	1.64	0.42
1:A:252:LEU:HD13	1:A:252:LEU:O	2.20	0.42
1:C:122:PHE:CE2	1:C:247[B]:MET:HE1	2.55	0.42
1:B:37:LYS:HG2	8:B:604:HOH:O	2.18	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
5:A:574:2PE:H271	6:B:575:PG4:H62	2.01	0.42
1:C:24:ILE:HA	1:C:25:PRO:HD3	1.95	0.42
1:D:26:LEU:HD23	8:D:681:HOH:O	2.20	0.42
1:A:97:ILE:C	1:A:98:LEU:HD12	2.40	0.41
1:A:170:THR:CG2	1:A:187:SER:HB2	2.50	0.41
1:A:231:VAL:O	1:A:248:SER:HA	2.20	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:C:272:PHE:CD1	1:C:272:PHE:N	2.88	0.41
1:A:131:ILE:HD13	1:A:200:LEU:HB2	2.02	0.41
1:B:206[A]:MET:HE1	1:B:212:ILE:HD12	2.02	0.41
1:D:171:VAL:N	1:D:190:LYS:CD	2.83	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:B:238:VAL:C	1:B:240:GLU:H	2.24	0.41
1:C:234:GLU:O	1:C:234:GLU:HG3	2.19	0.41
1:D:115:LEU:HD13	1:D:143:PRO:HB2	2.02	0.41
1:D:206[A]:MET:HE3	1:D:212:ILE:CD1	2.51	0.41
1:A:160:ARG:HE	1:A:160:ARG:HA	1.85	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: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:C:262:ILE:HG23	1:C:262:ILE:O	2.21	0.41
1:D:238:VAL:HA	1:D:241:ARG:NE	2.36	0.41
1:B:16:LEU:HD13	1:B:59:LEU:HD11	2.03	0.41
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.75	0.40
1:A:204:ASP:O	1:A:232:LEU:HB3	2.21	0.40
1:C:180:SER:O	1:C:182:ARG:N	2.54	0.40
1:C:206[A]:MET:HE2	1:C:212:ILE:CD1	2.51	0.40
1:D:121:LEU:O	1:D:121:LEU:HD23	2.22	0.40
1:A:130:GLU:O	1:A:198:ASN:HB3	2.20	0.40
1:B:135[A]:MET:HE3	1:B:219:LEU:HD21	2.03	0.40
1:C:256:ASN:HD22	1:C:259:GLU:CB	2.31	0.40
1:D:102:TYR:CD1	1:D:102:TYR:N	2.89	0.40
1:D:190:LYS:NZ	1:D:222:PHE:CZ	2.75	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
1:C:135[B]:MET:CE	1:C:215[B]:MET:HB3	2.52	0.40
1:D:255:ILE:HG23	1:D:255:ILE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/291 (94%)	258 (94%)	13 (5%)	3 (1%)	14	12
1	B	273/291 (94%)	262 (96%)	8 (3%)	3 (1%)	14	12
1	C	274/291 (94%)	265 (97%)	7 (3%)	2 (1%)	22	22
1	D	273/291 (94%)	258 (94%)	12 (4%)	3 (1%)	14	12
All	All	1094/1164 (94%)	1043 (95%)	40 (4%)	11 (1%)	15	14

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%)	27	34
1	B	237/250 (95%)	222 (94%)	15 (6%)	18	20
1	C	238/250 (95%)	225 (94%)	13 (6%)	21	26
1	D	237/250 (95%)	226 (95%)	11 (5%)	27	34
All	All	950/1000 (95%)	900 (95%)	50 (5%)	23	27



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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	D	571	-	15,15,15	1.09	0	18,20,20	0.74	0
7	1PE	D	577	-	15,15,15	0.58	0	14,14,14	0.35	0
2	SO4	B	589	-	4,4,4	0.27	0	6,6,6	0.14	0
3	EPE	A	570	-	15,15,15	1.24	2 (13%)	18,20,20	0.72	0
2	SO4	A	581	-	4,4,4	0.16	0	6,6,6	0.42	0
7	1PE	C	576	-	15,15,15	0.39	0	14,14,14	0.45	0
2	SO4	B	586	-	4,4,4	0.30	0	6,6,6	0.09	0
4	P6G	D	573	-	18,18,18	0.47	0	17,17,17	0.36	0
2	SO4	D	584	-	4,4,4	0.20	0	6,6,6	0.38	0
6	PG4	B	575	-	12,12,12	0.38	0	11,11,11	0.48	0
2	SO4	B	582	-	4,4,4	0.12	0	6,6,6	0.36	0
2	SO4	C	587	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	C	590	-	4,4,4	0.32	0	6,6,6	0.10	0
5	2PE	A	574	-	27,27,27	0.51	0	26,26,26	0.30	0
2	SO4	C	583	-	4,4,4	0.16	0	6,6,6	0.42	0
4	P6G	A	572	-	18,18,18	0.45	0	17,17,17	0.32	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	D	571	-	-	1/9/19/19	0/1/1/1
7	1PE	D	577	-	-	3/13/13/13	-
3	EPE	A	570	-	-	6/9/19/19	0/1/1/1
7	1PE	C	576	-	-	6/13/13/13	-
4	P6G	D	573	-	-	7/16/16/16	-
6	PG4	B	575	-	-	4/10/10/10	-
5	2PE	A	574	-	-	13/25/25/25	-
4	P6G	A	572	-	-	9/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	EPE	C10-S	2.51	1.81	1.77
3	A	570	EPE	C9-N1	2.01	1.52	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	570	EPE	C9-C10-S-O1S
3	A	570	EPE	C9-C10-S-O3S
7	C	576	1PE	OH4-C13-C23-OH3
5	A	574	2PE	O7-C8-C9-O10
5	A	574	2PE	O10-C11-C12-O13
5	A	574	2PE	O16-C17-C18-O19
7	D	577	1PE	OH6-C15-C25-OH5
4	A	572	P6G	O1-C2-C3-O4
5	A	574	2PE	O1-C2-C3-O4
5	A	574	2PE	O25-C26-C27-O28
5	A	574	2PE	O4-C5-C6-O7
7	C	576	1PE	OH5-C14-C24-OH4
6	B	575	PG4	O1-C1-C2-O2
7	C	576	1PE	OH2-C12-C22-OH3
3	A	570	EPE	N4-C7-C8-O8
7	D	577	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
4	A	572	P6G	O16-C17-C18-O19
4	D	573	P6G	O1-C2-C3-O4
4	D	573	P6G	C18-C17-O16-C15
5	A	574	2PE	C27-C26-O25-C24
4	A	572	P6G	C15-C14-O13-C12
4	D	573	P6G	C12-C11-O10-C9
5	A	574	2PE	C8-C9-O10-C11
5	A	574	2PE	C23-C24-O25-C26
4	A	572	P6G	C2-C3-O4-C5
5	A	574	2PE	C20-C21-O22-C23
5	A	574	2PE	C2-C3-O4-C5
5	A	574	2PE	C6-C5-O4-C3
4	A	572	P6G	C5-C6-O7-C8
3	A	570	EPE	C9-C10-S-O2S
6	B	575	PG4	C5-C6-O4-C7
4	A	572	P6G	C11-C12-O13-C14
7	C	576	1PE	C13-C23-OH3-C22
6	B	575	PG4	C1-C2-O2-C3
6	B	575	PG4	O2-C3-C4-O3
3	A	570	EPE	C8-C7-N4-C3
4	A	572	P6G	O4-C5-C6-O7
5	A	574	2PE	C11-C12-O13-C14
7	C	576	1PE	C24-C14-OH5-C25
3	A	570	EPE	C8-C7-N4-C5
4	A	572	P6G	C6-C5-O4-C3
7	D	577	1PE	C12-C22-OH3-C23
4	D	573	P6G	O10-C11-C12-O13
4	D	573	P6G	C15-C14-O13-C12
7	C	576	1PE	C23-C13-OH4-C24
4	A	572	P6G	C18-C17-O16-C15
4	D	573	P6G	C8-C9-O10-C11
4	D	573	P6G	C6-C5-O4-C3
3	D	571	EPE	C9-C10-S-O1S

There are no ring outliers.

8 monomers are involved in 31 short contacts:

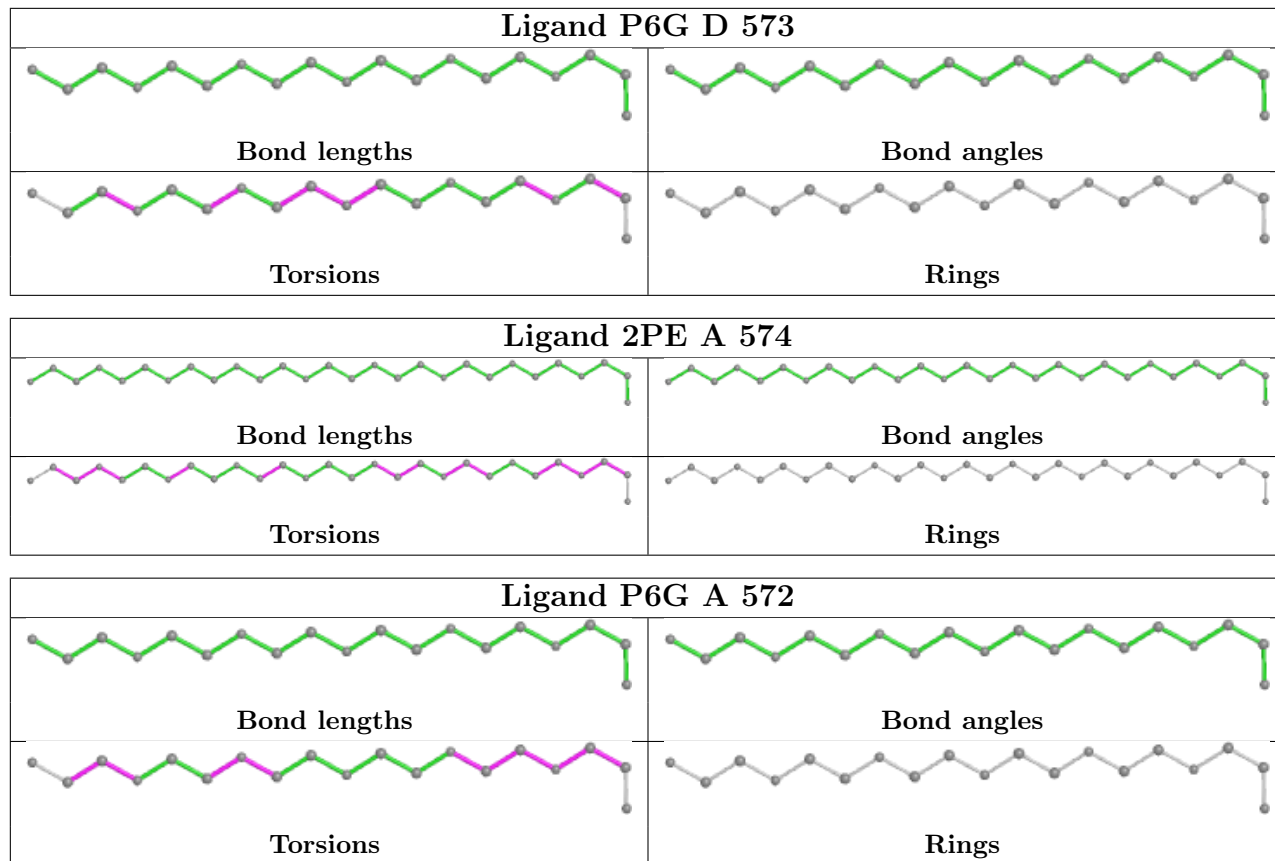
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	571	EPE	1	0
7	D	577	1PE	4	0
3	A	570	EPE	3	0
7	C	576	1PE	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	573	P6G	2	0
6	B	575	PG4	6	0
5	A	574	2PE	10	0
4	A	572	P6G	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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%)	0.62	45 (16%) <b>1</b> <b>1</b>	23, 46, 108, 163	0
1	B	269/291 (92%)	0.39	36 (13%) <b>3</b> <b>2</b>	23, 43, 94, 125	0
1	C	269/291 (92%)	0.28	26 (9%) <b>7</b> <b>6</b>	22, 39, 88, 115	0
1	D	270/291 (92%)	0.56	38 (14%) <b>2</b> <b>2</b>	24, 46, 97, 154	0
All	All	1078/1164 (92%)	0.46	145 (13%) <b>3</b> <b>2</b>	22, 43, 99, 163	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	11.0
1	B	179	SER	11.0
1	A	257	MET	10.3
1	D	257	MET	8.3
1	A	256	ASN	7.4
1	A	275	ASP	7.3
1	D	275	ASP	6.9
1	D	258	LYS	6.7
1	A	258	LYS	6.5
1	C	179	SER	6.3
1	C	180	SER	6.1
1	A	101	GLY	6.1
1	D	183	ILE	6.0
1	B	238	VAL	5.6
1	C	169	SER	5.4
1	C	168	GLY	5.4
1	A	180	SER	5.3
1	C	241	ARG	5.3
1	A	182	ARG	5.3
1	D	256	ASN	5.2
1	D	181	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	169	SER	5.1
1	A	185	THR	5.0
1	A	183	ILE	5.0
1	A	181	ASN	4.9
1	D	64	GLY	4.8
1	A	276	ASN	4.8
1	D	276	ASN	4.6
1	B	254	THR	4.6
1	A	260	LYS	4.5
1	C	274	LYS	4.5
1	A	100	GLY	4.5
1	D	182	ARG	4.4
1	A	179	SER	4.4
1	A	193[A]	MET	4.3
1	A	176	VAL	4.3
1	C	258	LYS	4.2
1	A	168	GLY	4.2
1	D	66	ALA	4.2
1	D	259	GLU	4.1
1	D	162	ASP	4.1
1	D	255	ILE	4.1
1	B	258	LYS	4.0
1	A	169	SER	3.9
1	A	259	GLU	3.9
1	C	206[A]	MET	3.7
1	C	247[A]	MET	3.7
1	B	206[A]	MET	3.7
1	A	162	ASP	3.6
1	D	185	THR	3.6
1	B	1	MET	3.6
1	C	178	GLY	3.6
1	D	247[A]	MET	3.6
1	B	168	GLY	3.6
1	B	180	SER	3.5
1	D	206[A]	MET	3.5
1	C	237	GLY	3.5
1	A	171	VAL	3.5
1	B	169	SER	3.5
1	D	180	SER	3.4
1	A	254	THR	3.4
1	B	239	ASP	3.3
1	B	178	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	261	SER	3.3
1	A	215[A]	MET	3.2
1	A	63	PRO	3.2
1	D	97	ILE	3.2
1	C	238	VAL	3.2
1	D	168	GLY	3.2
1	D	65	ALA	3.2
1	A	192	SER	3.2
1	A	274	LYS	3.1
1	A	97	ILE	3.1
1	C	215[A]	MET	3.1
1	D	260	LYS	3.1
1	C	135[A]	MET	3.0
1	D	179	SER	3.0
1	B	170	THR	2.9
1	B	241	ARG	2.9
1	B	237	GLY	2.9
1	A	247[A]	MET	2.8
1	B	247[A]	MET	2.8
1	D	274	LYS	2.8
1	D	193[A]	MET	2.8
1	D	62	VAL	2.8
1	A	135[A]	MET	2.8
1	B	135[A]	MET	2.8
1	C	193[A]	MET	2.7
1	C	239	ASP	2.7
1	B	102	TYR	2.7
1	B	240	GLU	2.7
1	D	135[A]	MET	2.7
1	A	206[A]	MET	2.7
1	A	190	LYS	2.6
1	D	99	PRO	2.6
1	A	184	GLN	2.6
1	B	255	ILE	2.6
1	B	195	THR	2.6
1	C	254	THR	2.6
1	C	202	ILE	2.6
1	B	257	MET	2.6
1	B	162	ASP	2.6
1	A	195	THR	2.6
1	B	259	GLU	2.6
1	D	171	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	100	GLY	2.6
1	B	97	ILE	2.5
1	D	170	THR	2.5
1	A	93	ASN	2.5
1	C	162	ASP	2.5
1	A	241	ARG	2.5
1	C	243	VAL	2.5
1	D	190	LYS	2.4
1	A	102	TYR	2.4
1	C	201	ILE	2.4
1	A	174	ASN	2.4
1	B	261	SER	2.4
1	D	161	LYS	2.3
1	C	229	ILE	2.3
1	D	3	PHE	2.3
1	B	274	LYS	2.3
1	C	257[A]	MET	2.3
1	B	182	ARG	2.3
1	A	99	PRO	2.3
1	D	2	LYS	2.3
1	B	231	VAL	2.3
1	A	2	LYS	2.2
1	A	161	LYS	2.2
1	B	193[A]	MET	2.2
1	A	186[A]	MET	2.2
1	B	215[A]	MET	2.2
1	A	4	ARG	2.1
1	C	240	GLU	2.1
1	B	85	GLN	2.1
1	B	262	ILE	2.1
1	D	215[A]	MET	2.1
1	C	194	LYS	2.1
1	B	89	GLN	2.1
1	A	191	ARG	2.1
1	B	260	LYS	2.1
1	C	230	GLY	2.0
1	B	194	LYS	2.0
1	D	63	PRO	2.0
1	B	256	ASN	2.0
1	D	195	THR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

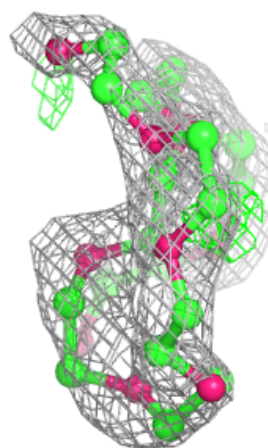
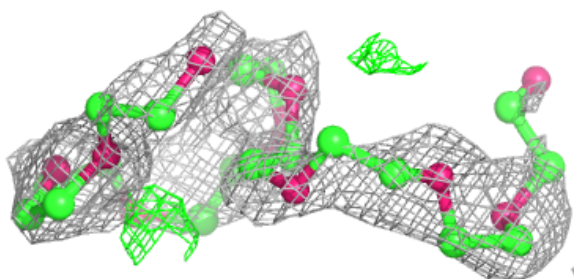
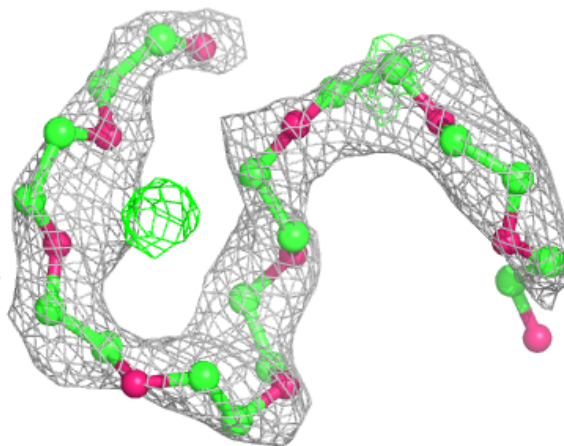
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	B	589	5/5	0.71	0.27	84,84,92,92	5
3	EPE	A	570	15/15	0.76	0.50	93,106,109,110	15
3	EPE	D	571	15/15	0.76	0.52	100,104,112,115	15
7	1PE	D	577	16/16	0.76	0.35	80,94,103,107	0
2	SO4	C	590	5/5	0.78	0.30	88,88,91,92	5
7	1PE	C	576	16/16	0.79	0.27	82,93,96,98	0
5	2PE	A	574	28/28	0.80	0.30	79,91,100,102	0
4	P6G	D	573	19/19	0.82	0.25	53,77,97,98	0
4	P6G	A	572	19/19	0.85	0.25	48,81,91,92	0
6	PG4	B	575	13/13	0.85	0.35	75,83,94,98	0
2	SO4	B	586	5/5	0.95	0.10	56,62,65,67	5
2	SO4	C	587	5/5	0.96	0.11	55,55,59,63	5
2	SO4	D	584	5/5	0.97	0.09	52,53,57,64	0
2	SO4	A	581	5/5	0.98	0.11	56,56,67,68	0
2	SO4	C	583	5/5	0.99	0.14	42,44,54,69	0
2	SO4	B	582	5/5	0.99	0.10	50,51,64,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

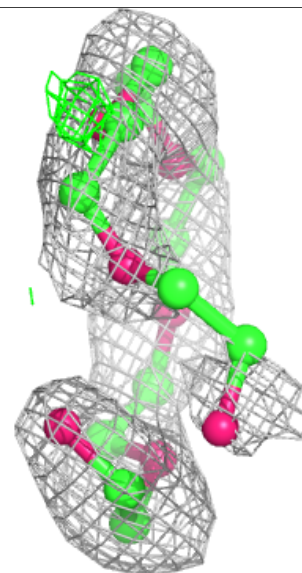
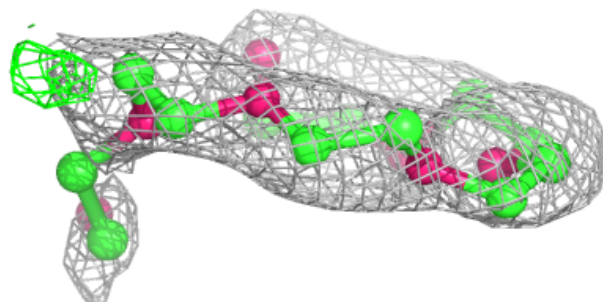
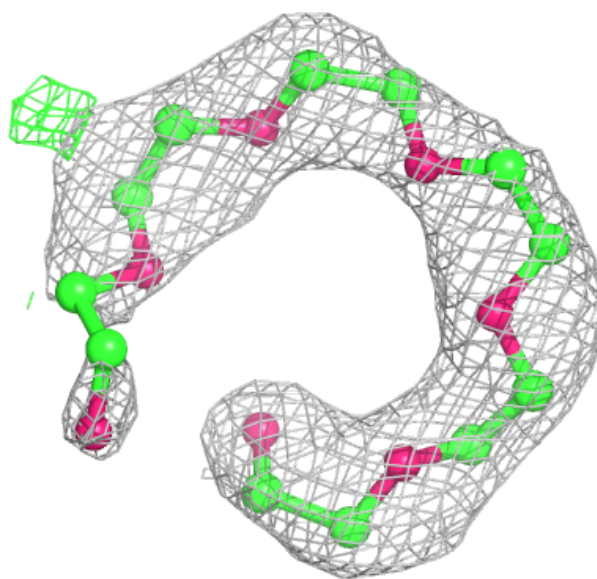
**Electron density around 2PE A 574:**

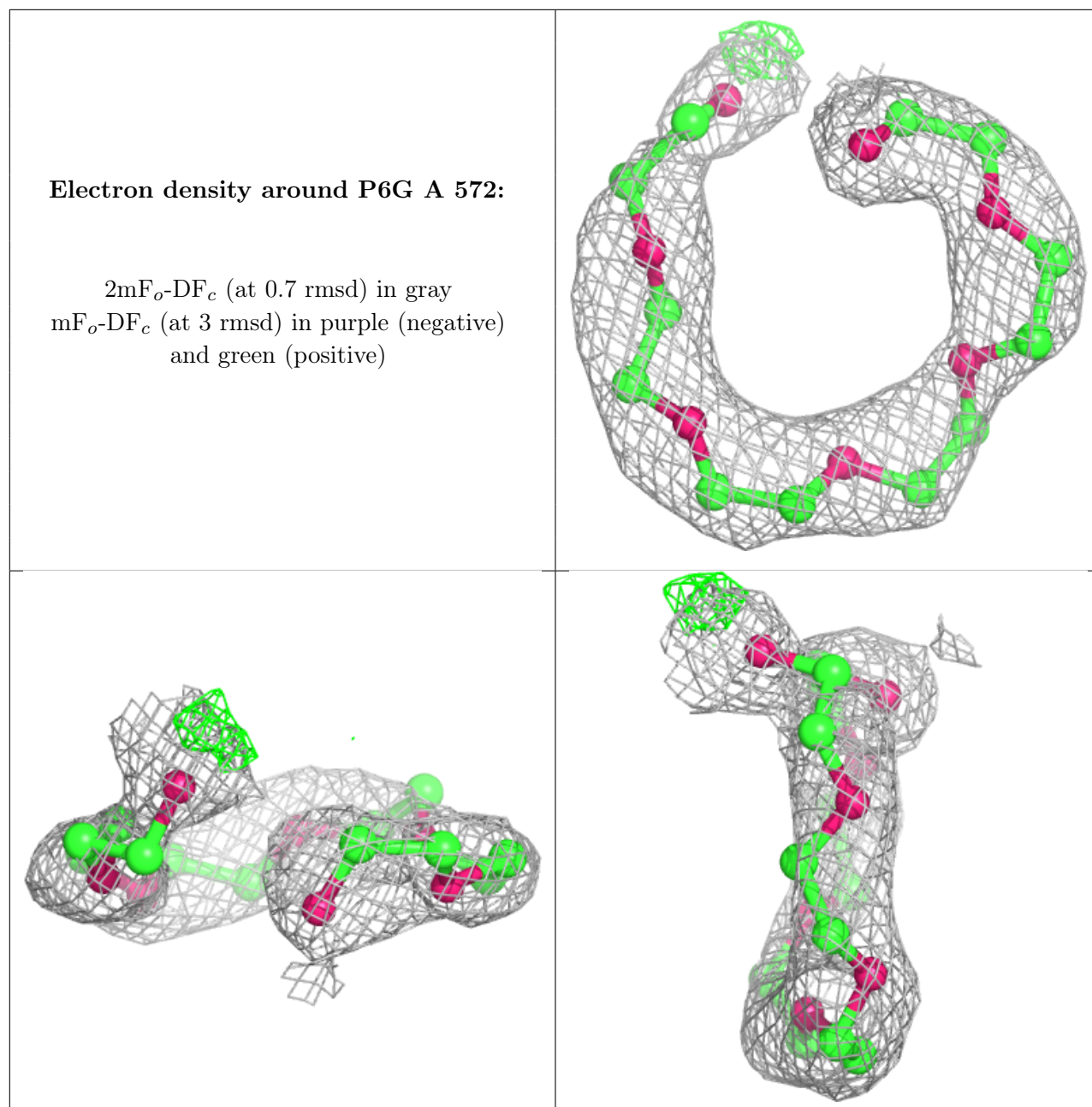
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P6G D 573:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.