



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 10:33 AM EDT

PDB ID : 2FXA
Title : Structure of the Protease Production Regulatory Protein hpr from *Bacillus subtilis*.
Authors : Cuff, M.E.; Skarina, T.; Edwards, A.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-02-03
Resolution : 2.40 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

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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

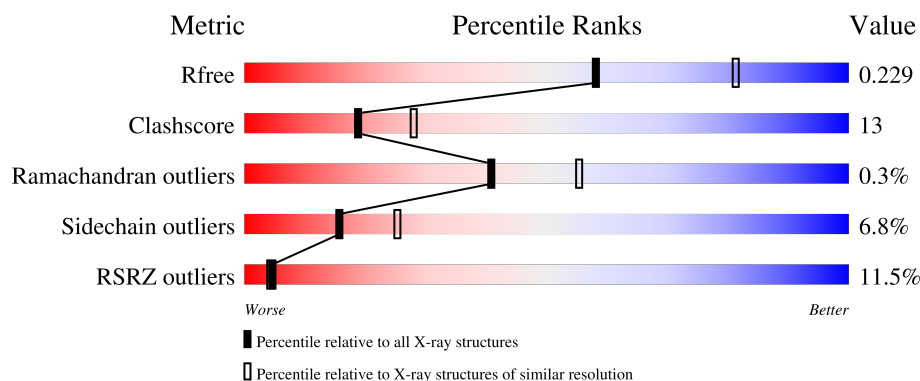
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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	207	
1	B	207	
1	C	207	
1	D	207	

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
2	EDO	A	207	-	-	X	-
2	EDO	B	207	-	-	X	-
2	EDO	D	206	-	-	X	-
3	1PE	D	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5953 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 Protease production regulatory protein hpr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	10	0
			1395	909	232	247	1	6			
1	B	180	Total	C	N	O	S	Se	0	4	0
			1527	988	253	279	1	6			
1	C	160	Total	C	N	O	S	Se	0	5	0
			1385	902	229	247	1	6			
1	D	156	Total	C	N	O	S	Se	0	5	0
			1352	884	218	243	1	6			

There are 44 discrepancies between the modelled and reference sequences:

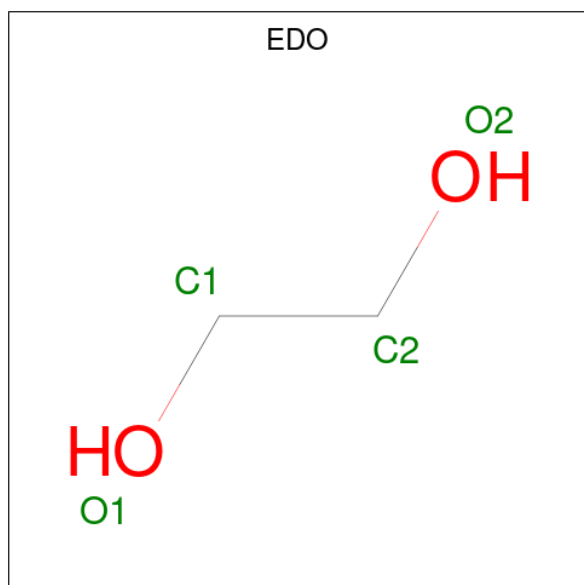
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P11065
A	0	HIS	-	CLONING ARTIFACT	UNP P11065
A	1	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	20	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	72	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	148	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	149	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	151	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	161	MSE	MET	MODIFIED RESIDUE	UNP P11065
A	204	GLY	-	CLONING ARTIFACT	UNP P11065
A	205	SER	-	CLONING ARTIFACT	UNP P11065
B	-1	GLY	-	CLONING ARTIFACT	UNP P11065
B	0	HIS	-	CLONING ARTIFACT	UNP P11065
B	1	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	20	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	72	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	148	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	149	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	151	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	161	MSE	MET	MODIFIED RESIDUE	UNP P11065
B	204	GLY	-	CLONING ARTIFACT	UNP P11065

Continued on next page...

Continued from previous page...

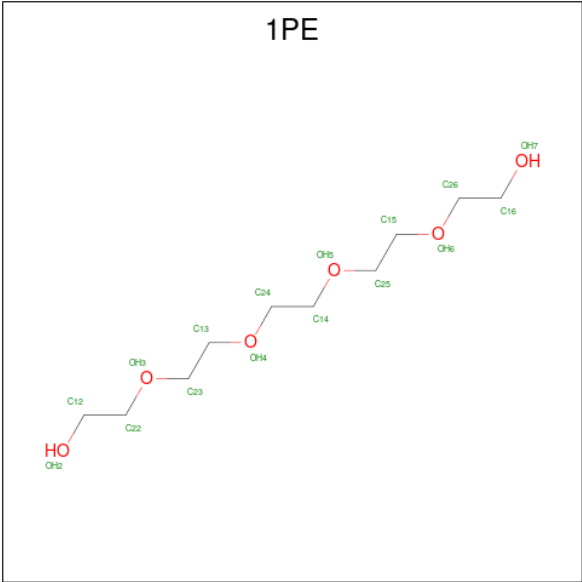
Chain	Residue	Modelled	Actual	Comment	Reference
B	205	SER	-	CLONING ARTIFACT	UNP P11065
C	-1	GLY	-	CLONING ARTIFACT	UNP P11065
C	0	HIS	-	CLONING ARTIFACT	UNP P11065
C	1	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	20	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	72	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	148	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	149	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	151	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	161	MSE	MET	MODIFIED RESIDUE	UNP P11065
C	204	GLY	-	CLONING ARTIFACT	UNP P11065
C	205	SER	-	CLONING ARTIFACT	UNP P11065
D	-1	GLY	-	CLONING ARTIFACT	UNP P11065
D	0	HIS	-	CLONING ARTIFACT	UNP P11065
D	1	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	20	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	72	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	148	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	149	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	151	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	161	MSE	MET	MODIFIED RESIDUE	UNP P11065
D	204	GLY	-	CLONING ARTIFACT	UNP P11065
D	205	SER	-	CLONING ARTIFACT	UNP P11065

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



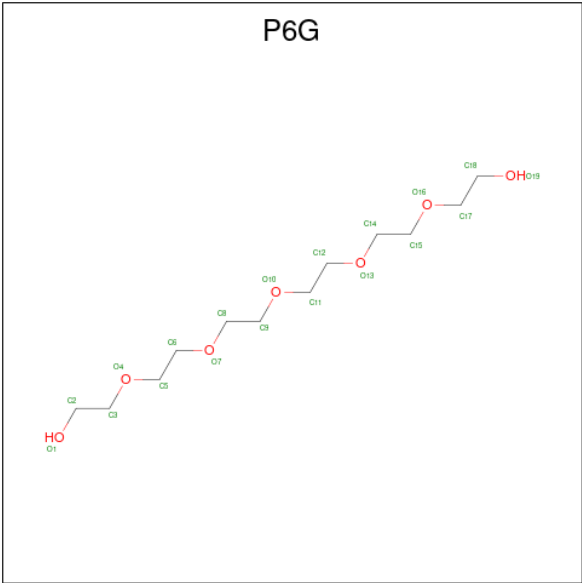
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0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

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		

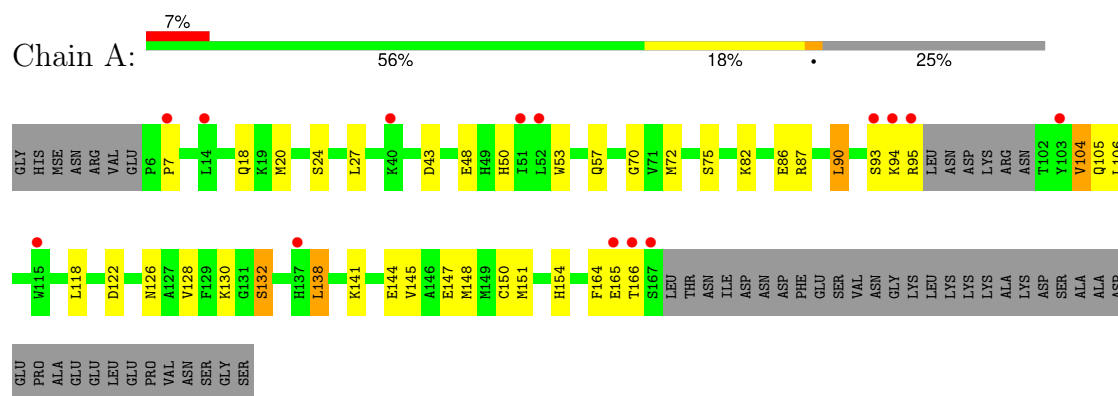
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	62	Total	O	0	0
			62	62		
6	C	33	Total	O	0	0
			33	33		
6	D	33	Total	O	0	0
			33	33		

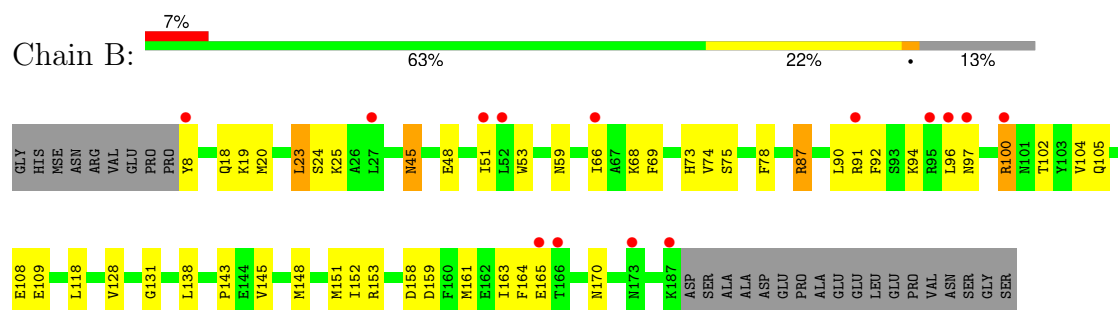
3 Residue-property plots

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.

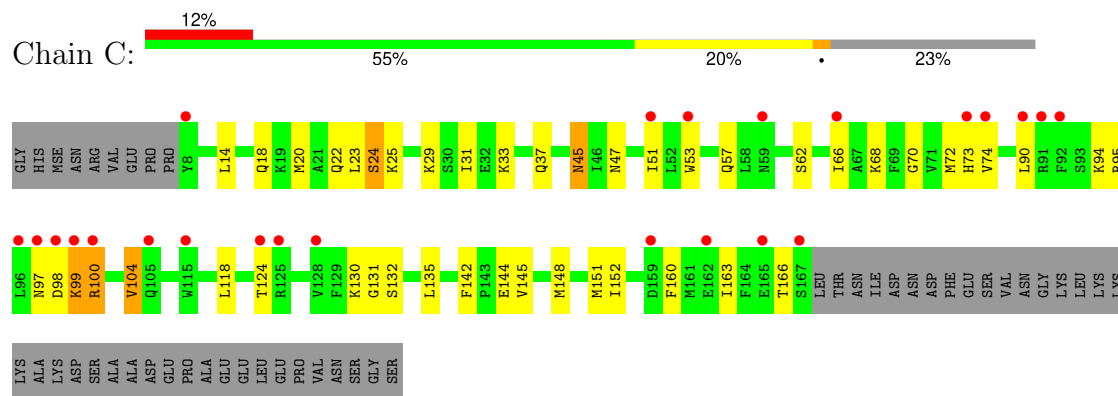
- Molecule 1: Protease production regulatory protein hpr



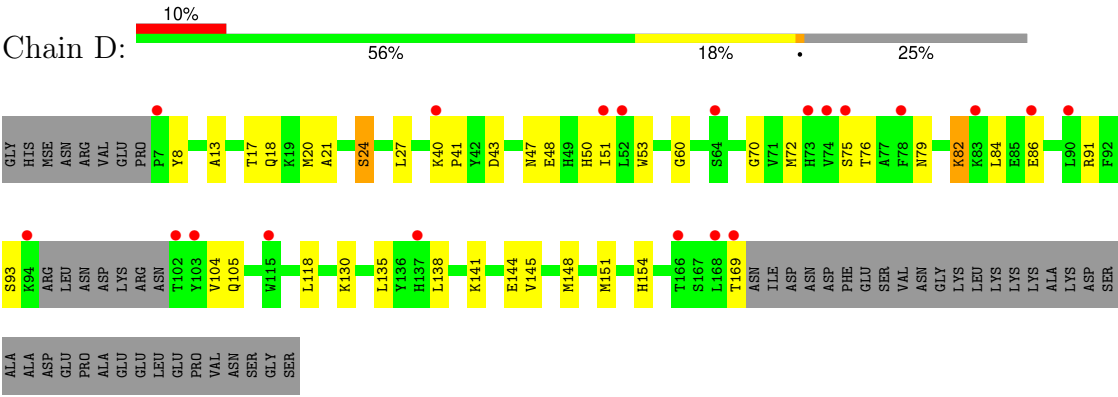
- Molecule 1: Protease production regulatory protein hpr



- Molecule 1: Protease production regulatory protein hpr



- Molecule 1: Protease production regulatory protein hpr



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.27Å 79.91Å 131.24Å 90.00° 100.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 19.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.40) 97.3 (19.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.234 0.208 , 0.229	Depositor DCC
R_{free} test set	2095 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5953	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, P6G, 1PE, PGE

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	0.85	0/1441	0.77	1/1934 (0.1%)
1	B	0.80	0/1568	0.75	0/2100
1	C	0.67	1/1428 (0.1%)	0.80	2/1916 (0.1%)
1	D	0.68	0/1387	0.67	1/1863 (0.1%)
All	All	0.76	1/5824 (0.0%)	0.75	4/7813 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	ARG	NE-CZ	6.48	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	ARG	NE-CZ-NH1	-16.16	112.22	120.30
1	C	95	ARG	NE-CZ-NH2	10.91	125.75	120.30
1	D	91	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	90	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1395	0	1344	35	0
1	B	1527	0	1504	52	0
1	C	1385	0	1348	49	0
1	D	1352	0	1298	38	0
2	A	24	0	36	13	0
2	B	16	0	24	8	0
2	C	8	0	12	0	0
2	D	8	0	12	8	0
3	A	16	0	22	3	0
3	D	16	0	22	7	0
4	B	19	0	26	0	0
5	C	10	0	14	0	0
6	A	49	0	0	0	0
6	B	62	0	0	4	0
6	C	33	0	0	6	0
6	D	33	0	0	1	0
All	All	5953	0	5662	150	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 13.

All (150) 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:C:132:SER:HB3	6:C:332:HOH:O	1.08	1.24
1:A:148:MSE:HB2	2:A:207:EDO:H11	1.49	0.94
1:A:18:GLN:NE2	1:B:53:TRP:CZ2	2.36	0.93
1:A:18:GLN:HE22	1:B:53:TRP:HZ2	1.21	0.88
1:C:23:LEU:HD13	1:D:148:MSE:HE3	1.55	0.88
1:A:126:ASN:HD22	3:A:304:1PE:H152	1.38	0.88
1:A:164:PHE:CZ	1:B:23:LEU:HD13	2.08	0.87
2:A:207:EDO:H22	1:B:148:MSE:HB2	1.65	0.78
1:A:105[B]:GLN:HE21	1:A:106:LEU:H	1.31	0.77
1:C:148:MSE:HE3	2:D:206:EDO:H12	1.67	0.77
1:A:18:GLN:NE2	1:B:53:TRP:HZ2	1.77	0.77
1:C:23:LEU:HD13	1:D:148:MSE:CE	2.18	0.73
1:B:45:ASN:C	1:B:45:ASN:HD22	1.90	0.73
1:B:20:MSE:HE2	1:B:151:MSE:HE1	1.71	0.73
1:C:148:MSE:HE2	1:D:148:MSE:SE	2.40	0.72
1:D:145:VAL:CG2	1:D:148:MSE:HE2	2.20	0.71
1:A:122:ASP:H	3:A:304:1PE:H162	1.56	0.71
1:C:18:GLN:HG3	3:D:303:1PE:H232	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:CG	1:B:87:ARG:HH21	2.04	0.70
1:A:154[B]:HIS:CD2	1:B:131:GLY:HA2	2.27	0.69
1:C:90:LEU:HD13	1:C:104:VAL:HG11	1.74	0.68
1:D:8:TYR:HB2	2:D:210:EDO:H12	1.77	0.67
1:D:145:VAL:HG21	1:D:148:MSE:CE	2.24	0.67
1:C:53[A]:TRP:HE1	1:C:57:GLN:HE21	1.42	0.67
1:C:99:LYS:HG3	1:C:100:ARG:N	2.10	0.66
1:C:73:HIS:HD2	6:C:306:HOH:O	1.77	0.65
1:D:148:MSE:H	2:D:206:EDO:H22	1.60	0.65
1:C:132:SER:CB	6:C:332:HOH:O	1.91	0.65
1:B:74:VAL:HG12	2:B:207:EDO:O2	1.98	0.63
1:D:75:SER:O	1:D:79:ASN:HB2	1.97	0.63
1:A:164:PHE:HZ	1:B:23:LEU:HD13	1.62	0.63
1:B:73:HIS:HD2	1:B:75:SER:H	1.46	0.61
1:B:90:LEU:HD22	1:B:104:VAL:HG13	1.81	0.61
1:A:148:MSE:HA	1:A:151:MSE:HE2	1.82	0.61
1:C:18:GLN:NE2	3:D:303:1PE:OH4	2.33	0.61
1:B:68:LYS:HE2	1:B:159:ASP:HB3	1.84	0.60
1:D:20:MSE:O	1:D:24:SER:HB3	2.02	0.60
1:D:53:TRP:NE1	3:D:303:1PE:H221	2.16	0.59
1:C:73:HIS:CD2	6:C:306:HOH:O	2.53	0.59
1:C:124:THR:O	1:C:130:LYS:HD2	2.02	0.59
1:A:145:VAL:HB	2:A:207:EDO:H12	1.85	0.59
1:D:145:VAL:HG21	1:D:148:MSE:HE2	1.83	0.59
1:B:75:SER:CB	2:B:207:EDO:H12	2.34	0.58
1:C:45:ASN:HD22	1:C:47:ASN:H	1.53	0.56
1:A:145:VAL:CB	2:A:207:EDO:H12	2.35	0.56
1:B:75:SER:HA	2:B:207:EDO:H12	1.87	0.56
1:C:70:GLY:HA3	1:C:72:MSE:HE3	1.87	0.56
1:C:14:LEU:HD12	1:C:18:GLN:OE1	2.04	0.56
1:B:8:TYR:N	6:B:356:HOH:O	2.38	0.56
1:C:20:MSE:O	1:C:24:SER:HB3	2.06	0.55
1:B:73:HIS:CD2	1:B:75:SER:H	2.24	0.55
1:C:99:LYS:HG3	1:C:100:ARG:H	1.72	0.55
1:B:87:ARG:HH21	1:B:87:ARG:HG2	1.72	0.54
1:A:48:GLU:OE2	1:A:87[A]:ARG:NH2	2.41	0.54
1:B:78:PHE:CB	2:B:207:EDO:H21	2.38	0.53
1:A:20:MSE:O	1:A:24:SER:HB3	2.08	0.53
2:A:207:EDO:H21	1:B:145:VAL:CB	2.38	0.53
1:B:45:ASN:C	1:B:45:ASN:ND2	2.62	0.53
1:A:27:LEU:HB2	1:B:152:ILE:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:VAL:HG21	1:D:148:MSE:HE1	1.90	0.53
1:C:94:LYS:HB3	1:C:97:ASN:HD22	1.74	0.53
1:D:148:MSE:H	2:D:206:EDO:C2	2.20	0.53
1:B:59[A]:ASN:HD21	1:B:170:ASN:HD21	1.57	0.52
1:B:91:ARG:NH2	6:B:363:HOH:O	2.42	0.52
1:D:60:GLY:HA2	1:D:104:VAL:O	2.09	0.52
1:B:20:MSE:O	1:B:24:SER:HB3	2.10	0.52
2:A:207:EDO:H21	1:B:145:VAL:HB	1.92	0.52
1:B:78:PHE:HB3	2:B:207:EDO:H21	1.92	0.52
1:A:20:MSE:HE2	1:A:151:MSE:HE1	1.92	0.51
2:A:207:EDO:H21	1:B:145:VAL:HA	1.92	0.51
1:B:19:LYS:HB2	2:B:206:EDO:C1	2.40	0.51
1:C:151:MSE:HE1	1:D:145:VAL:CG1	2.40	0.51
1:C:45:ASN:HD22	1:C:47:ASN:N	2.07	0.51
1:C:99:LYS:NZ	1:C:99:LYS:HB2	2.24	0.51
1:B:87:ARG:CG	1:B:87:ARG:NH2	2.71	0.51
1:C:22:GLN:HB2	3:D:303:1PE:C12	2.41	0.50
1:C:22:GLN:HE22	1:D:50:HIS:HE2	1.60	0.50
1:B:45:ASN:ND2	1:B:48:GLU:H	2.10	0.50
1:C:160:PHE:O	1:C:163:ILE:HG22	2.12	0.50
1:D:130:LYS:NZ	6:D:336:HOH:O	2.41	0.49
1:D:145:VAL:HG12	2:D:206:EDO:H11	1.94	0.49
1:D:148:MSE:N	2:D:206:EDO:H22	2.28	0.49
1:A:50:HIS:HD1	1:B:25:LYS:HZ3	1.61	0.48
1:B:87:ARG:HG2	1:B:87:ARG:NH2	2.28	0.48
2:A:207:EDO:H21	1:B:145:VAL:CA	2.43	0.48
1:A:145:VAL:CA	2:A:207:EDO:H12	2.43	0.48
1:B:100:ARG:HE	1:B:100:ARG:HB3	1.57	0.47
1:C:151:MSE:HE1	1:D:145:VAL:HG11	1.96	0.47
1:A:164:PHE:CZ	1:B:23:LEU:CD1	2.91	0.47
1:B:19:LYS:HB2	2:B:206:EDO:H11	1.96	0.47
6:C:332:HOH:O	1:D:151:MSE:SE	2.83	0.47
1:A:43:ASP:O	1:A:87[A]:ARG:NH1	2.47	0.47
1:A:53:TRP:HE1	1:A:57:GLN:HE21	1.61	0.47
1:A:164:PHE:C	1:A:166:THR:H	2.17	0.46
1:A:147:GLU:HB2	2:A:207:EDO:O1	2.16	0.46
1:C:33:LYS:O	1:C:37[B]:GLN:HG2	2.16	0.46
1:C:74:VAL:HG21	1:C:100:ARG:HB3	1.97	0.45
1:A:150:CYS:O	1:A:154[A]:HIS:HD2	2.00	0.45
1:C:18:GLN:HG3	3:D:303:1PE:H222	1.99	0.44
1:A:82:LYS:O	1:A:86[A]:GLU:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HA	2:A:207:EDO:H12	1.99	0.44
1:B:153[A]:ARG:NE	1:B:158:ASP:OD1	2.38	0.44
1:B:108:GLU:HG2	1:B:109[A]:GLU:OE2	2.17	0.44
1:C:14:LEU:CD1	1:C:18:GLN:OE1	2.65	0.44
1:C:25:LYS:NZ	1:D:47:ASN:ND2	2.66	0.44
1:A:126:ASN:ND2	3:A:304:1PE:H152	2.18	0.44
1:C:131:GLY:HA2	1:D:154[B]:HIS:CD2	2.52	0.44
1:C:152:ILE:HD11	1:D:27:LEU:HB2	2.00	0.44
1:C:68:LYS:NZ	6:C:304:HOH:O	2.49	0.43
2:A:213:EDO:H21	1:B:143:PRO:HA	1.99	0.43
1:B:45:ASN:HB2	6:B:338:HOH:O	2.17	0.43
1:C:145:VAL:CG1	1:D:151:MSE:HE1	2.48	0.43
1:B:59[A]:ASN:ND2	1:B:170:ASN:HD21	2.16	0.43
1:A:128:VAL:O	1:A:132:SER:HB3	2.19	0.43
1:C:22:GLN:HB2	3:D:303:1PE:H121	2.00	0.43
1:B:75:SER:CA	2:B:207:EDO:H12	2.49	0.42
1:A:50:HIS:HD1	1:B:25:LYS:NZ	2.17	0.42
1:D:53:TRP:CD1	3:D:303:1PE:H221	2.54	0.42
1:B:161:MSE:O	1:B:164:PHE:HD1	2.02	0.42
1:C:142:PHE:CZ	2:D:210:EDO:H11	2.54	0.42
1:D:40:LYS:HB3	1:D:41:PRO:HD3	2.00	0.42
1:D:51:ILE:HG13	1:D:72:MSE:HE1	2.01	0.42
1:A:90:LEU:HD22	1:A:104:VAL:HG13	2.01	0.42
1:C:53[A]:TRP:HD1	1:C:57:GLN:HG2	1.85	0.42
1:D:82:LYS:O	1:D:86:GLU:HG3	2.19	0.42
1:D:145:VAL:CG2	1:D:148:MSE:CE	2.88	0.42
1:C:45:ASN:ND2	1:C:47:ASN:H	2.17	0.42
1:A:138:LEU:HD11	1:C:135:LEU:HD23	2.02	0.42
1:A:144[B]:GLU:OE1	2:A:208:EDO:O2	2.38	0.42
1:A:126:ASN:O	1:A:130:LYS:HG3	2.20	0.41
1:C:51:ILE:HG12	1:C:66:ILE:CG2	2.50	0.41
1:B:51:ILE:HG12	1:B:66:ILE:HG21	2.01	0.41
1:B:128:VAL:HG23	6:B:316:HOH:O	2.19	0.41
1:C:148:MSE:HA	1:C:151:MSE:HE3	2.02	0.41
1:C:47:ASN:O	1:C:51:ILE:HG13	2.20	0.41
1:B:92:PHE:HD1	1:B:102:THR:CG2	2.34	0.41
1:D:48:GLU:HB3	1:D:84:LEU:HD21	2.03	0.41
1:D:138:LEU:HD12	1:D:138:LEU:HA	1.64	0.41
1:C:31:ILE:HD13	1:D:21:ALA:HA	2.03	0.41
1:D:13:ALA:O	1:D:17:THR:HG23	2.20	0.41
1:C:62:SER:O	1:C:66:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLY:HA3	1:D:72:MSE:HE3	2.03	0.41
1:C:94:LYS:HB3	1:C:97:ASN:ND2	2.35	0.40
1:C:18:GLN:HG2	1:D:53:TRP:CH2	2.56	0.40
1:B:19:LYS:HG2	1:B:23:LEU:HD22	2.03	0.40
1:B:69:PHE:CD2	1:B:163:ILE:HB	2.57	0.40
1:B:138:LEU:HD21	1:D:135:LEU:HD23	2.03	0.40
1:A:70:GLY:HA3	1:A:72:MSE:HE3	2.04	0.40
1:C:25:LYS:O	1:C:29:LYS:HG2	2.22	0.40
1:D:145:VAL:CA	2:D:206:EDO:H21	2.51	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	162/207 (78%)	157 (97%)	3 (2%)	2 (1%)	13	19
1	B	182/207 (88%)	177 (97%)	5 (3%)	0	100	100
1	C	163/207 (79%)	159 (98%)	4 (2%)	0	100	100
1	D	157/207 (76%)	153 (98%)	4 (2%)	0	100	100
All	All	664/828 (80%)	646 (97%)	16 (2%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLU
1	A	7	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/177 (85%)	141 (94%)	9 (6%)	19	31
1	B	166/177 (94%)	155 (93%)	11 (7%)	16	26
1	C	149/177 (84%)	139 (93%)	10 (7%)	16	26
1	D	145/177 (82%)	133 (92%)	12 (8%)	11	17
All	All	610/708 (86%)	568 (93%)	42 (7%)	16	25

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	A	93	SER
1	A	94	LYS
1	A	95	ARG
1	A	104	VAL
1	A	118	LEU
1	A	132	SER
1	A	138	LEU
1	A	141	LYS
1	B	18	GLN
1	B	23	LEU
1	B	45	ASN
1	B	87	ARG
1	B	94	LYS
1	B	96	LEU
1	B	97	ASN
1	B	100	ARG
1	B	105	GLN
1	B	118	LEU
1	B	165	GLU
1	C	24	SER
1	C	45	ASN
1	C	98	ASP
1	C	99	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100	ARG
1	C	104	VAL
1	C	118	LEU
1	C	144[A]	GLU
1	C	144[B]	GLU
1	C	166	THR
1	D	18	GLN
1	D	24	SER
1	D	43	ASP
1	D	76	THR
1	D	82	LYS
1	D	93	SER
1	D	105	GLN
1	D	118	LEU
1	D	141	LYS
1	D	144[A]	GLU
1	D	144[B]	GLU
1	D	169	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	36	GLN
1	A	47	ASN
1	B	18	GLN
1	B	22	GLN
1	B	45	ASN
1	B	73	HIS
1	B	154	HIS
1	C	22	GLN
1	C	45	ASN
1	C	47	ASN
1	C	57	GLN
1	C	97	ASN
1	D	22	GLN
1	D	47	ASN

5.3.3 RNA ⓘ

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](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	B	208	-	3,3,3	0.36	0	2,2,2	0.47	0
2	EDO	C	208	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	A	208	-	3,3,3	0.35	0	2,2,2	0.81	0
3	1PE	D	303	-	15,15,15	0.86	0	14,14,14	0.96	0
2	EDO	D	210	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	D	206	-	3,3,3	0.10	0	2,2,2	0.97	0
2	EDO	A	206	-	3,3,3	0.35	0	2,2,2	0.91	0
2	EDO	B	206	-	3,3,3	0.52	0	2,2,2	0.27	0
2	EDO	C	209	-	3,3,3	0.40	0	2,2,2	0.57	0
2	EDO	A	213	-	3,3,3	0.53	0	2,2,2	0.50	0
2	EDO	A	207	-	3,3,3	0.40	0	2,2,2	0.97	0
2	EDO	A	212	-	3,3,3	0.54	0	2,2,2	0.29	0
5	PGE	C	301	-	9,9,9	0.73	0	8,8,8	0.92	0
2	EDO	B	211	-	3,3,3	0.54	0	2,2,2	0.42	0
2	EDO	A	214	-	3,3,3	0.40	0	2,2,2	0.42	0
4	P6G	B	302	-	18,18,18	0.66	0	17,17,17	0.43	0
2	EDO	B	207	-	3,3,3	0.33	0	2,2,2	0.54	0
3	1PE	A	304	-	15,15,15	1.09	1 (6%)	14,14,14	1.31	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	208	-	-	0/1/1/1	-
2	EDO	C	208	-	-	0/1/1/1	-
2	EDO	A	208	-	-	1/1/1/1	-
3	1PE	D	303	-	-	9/13/13/13	-
2	EDO	D	210	-	-	0/1/1/1	-
2	EDO	D	206	-	-	1/1/1/1	-
2	EDO	A	206	-	-	1/1/1/1	-
2	EDO	B	206	-	-	1/1/1/1	-
2	EDO	C	209	-	-	1/1/1/1	-
2	EDO	A	213	-	-	1/1/1/1	-
2	EDO	A	207	-	-	0/1/1/1	-
2	EDO	A	212	-	-	1/1/1/1	-
5	PGE	C	301	-	-	2/7/7/7	-
2	EDO	B	211	-	-	1/1/1/1	-
2	EDO	A	214	-	-	0/1/1/1	-
4	P6G	B	302	-	-	9/16/16/16	-
2	EDO	B	207	-	-	0/1/1/1	-
3	1PE	A	304	-	-	7/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	1PE	OH5-C25	2.08	1.51	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	1PE	OH5-C25-C15	2.58	122.11	110.35
3	A	304	1PE	OH4-C13-C23	2.46	121.55	110.35

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	1PE	C23-C13-OH4-C24
3	A	304	1PE	C13-C23-OH3-C22
3	A	304	1PE	C24-C14-OH5-C25
3	A	304	1PE	OH6-C15-C25-OH5
3	D	303	1PE	OH4-C13-C23-OH3
3	D	303	1PE	OH7-C16-C26-OH6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	211	EDO	O1-C1-C2-O2
2	C	209	EDO	O1-C1-C2-O2
2	D	206	EDO	O1-C1-C2-O2
4	B	302	P6G	O7-C8-C9-O10
4	B	302	P6G	O4-C5-C6-O7
4	B	302	P6G	C14-C15-O16-C17
3	D	303	1PE	C13-C23-OH3-C22
4	B	302	P6G	C2-C3-O4-C5
3	D	303	1PE	C25-C15-OH6-C26
4	B	302	P6G	C12-C11-O10-C9
3	A	304	1PE	C16-C26-OH6-C15
3	A	304	1PE	OH2-C12-C22-OH3
3	D	303	1PE	C16-C26-OH6-C15
5	C	301	PGE	C4-C3-O2-C2
4	B	302	P6G	C6-C5-O4-C3
2	B	206	EDO	O1-C1-C2-O2
2	A	212	EDO	O1-C1-C2-O2
4	B	302	P6G	C8-C9-O10-C11
4	B	302	P6G	C18-C17-O16-C15
2	A	206	EDO	O1-C1-C2-O2
2	A	213	EDO	O1-C1-C2-O2
3	D	303	1PE	C15-C25-OH5-C14
3	D	303	1PE	OH6-C15-C25-OH5
3	A	304	1PE	C25-C15-OH6-C26
5	C	301	PGE	O2-C3-C4-O3
2	A	208	EDO	O1-C1-C2-O2
3	D	303	1PE	OH5-C14-C24-OH4
4	B	302	P6G	O10-C11-C12-O13
3	D	303	1PE	C14-C24-OH4-C13

There are no ring outliers.

9 monomers are involved in 39 short contacts:

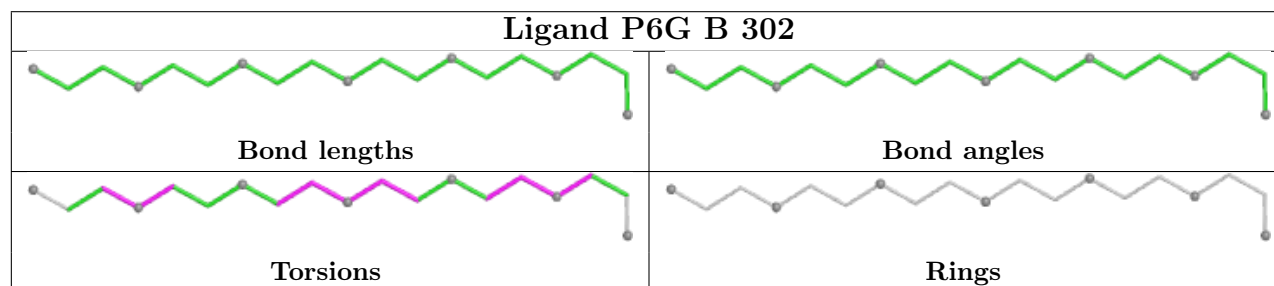
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	208	EDO	1	0
3	D	303	1PE	7	0
2	D	210	EDO	2	0
2	D	206	EDO	6	0
2	B	206	EDO	2	0
2	A	213	EDO	1	0
2	A	207	EDO	11	0
2	B	207	EDO	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	1PE	3	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/207 (72%)	0.63	14 (9%) 8 8	55, 62, 77, 97	0
1	B	174/207 (84%)	0.49	14 (8%) 12 11	54, 63, 81, 91	0
1	C	154/207 (74%)	0.79	24 (15%) 2 1	52, 63, 74, 88	0
1	D	150/207 (72%)	0.84	20 (13%) 3 3	51, 62, 78, 96	0
All	All	628/828 (75%)	0.68	72 (11%) 4 4	51, 63, 79, 97	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	LYS	8.3
1	B	8	TYR	6.9
1	C	96	LEU	6.7
1	A	167	SER	5.8
1	A	103	TYR	5.6
1	C	115	TRP	5.5
1	C	8	TYR	5.4
1	D	78	PHE	5.3
1	D	7	PRO	5.0
1	D	73	HIS	4.8
1	C	98	ASP	4.7
1	A	95	ARG	4.7
1	D	115[A]	TRP	4.5
1	D	168	LEU	4.4
1	C	97	ASN	4.3
1	C	91	ARG	4.3
1	D	169	THR	4.2
1	A	137[A]	HIS	4.1
1	A	7	PRO	4.0
1	B	51	ILE	4.0
1	C	74	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	74	VAL	3.8
1	B	165	GLU	3.8
1	C	105	GLN	3.7
1	B	100	ARG	3.6
1	D	103	TYR	3.5
1	A	93	SER	3.5
1	C	167	SER	3.5
1	A	94	LYS	3.4
1	C	90	LEU	3.4
1	B	166	THR	3.3
1	D	51	ILE	3.2
1	C	73	HIS	3.2
1	C	59	ASN	3.2
1	C	100	ARG	3.2
1	C	124	THR	3.1
1	A	166	THR	3.1
1	A	51	ILE	3.0
1	D	102	THR	3.0
1	D	40	LYS	3.0
1	B	97	ASN	2.8
1	A	40	LYS	2.8
1	D	64	SER	2.8
1	B	187	LYS	2.8
1	B	173	ASN	2.8
1	B	95	ARG	2.8
1	A	115[A]	TRP	2.7
1	B	96	LEU	2.7
1	C	51	ILE	2.7
1	B	91	ARG	2.7
1	B	66	ILE	2.5
1	D	86	GLU	2.5
1	D	75	SER	2.5
1	C	92	PHE	2.5
1	C	125[A]	ARG	2.4
1	D	52	LEU	2.4
1	C	162	GLU	2.3
1	C	53[A]	TRP	2.3
1	C	66	ILE	2.3
1	A	165	GLU	2.3
1	B	52	LEU	2.3
1	D	137[A]	HIS	2.2
1	D	90	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	2.2
1	B	27	LEU	2.2
1	D	83	LYS	2.1
1	A	52	LEU	2.1
1	C	159	ASP	2.1
1	C	128	VAL	2.1
1	D	166	THR	2.1
1	C	165	GLU	2.1
1	C	99	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

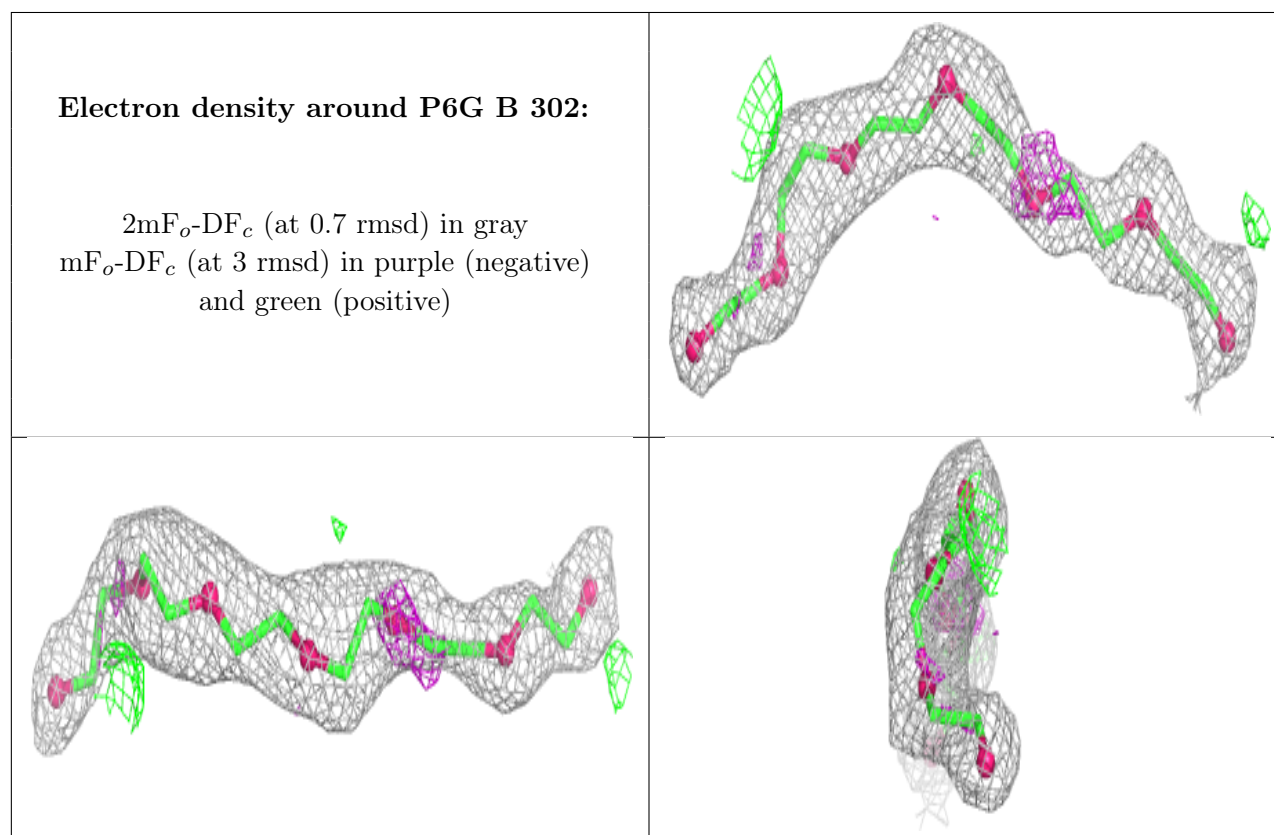
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	212	4/4	0.55	0.32	92,92,93,93	0
2	EDO	D	210	4/4	0.77	0.35	81,82,82,82	0
3	1PE	D	303	16/16	0.78	0.26	72,77,86,87	0
2	EDO	C	209	4/4	0.83	0.29	80,80,81,81	0
2	EDO	B	208	4/4	0.86	0.22	76,77,78,79	0
4	P6G	B	302	19/19	0.86	0.19	65,69,87,87	0
3	1PE	A	304	16/16	0.87	0.20	64,71,74,78	0
5	PGE	C	301	10/10	0.88	0.16	77,81,87,88	0
2	EDO	B	206	4/4	0.89	0.63	72,76,76,79	0
2	EDO	A	214	4/4	0.89	0.13	64,67,69,73	0
2	EDO	B	211	4/4	0.91	0.36	67,68,71,71	0
2	EDO	C	208	4/4	0.92	0.12	65,67,68,68	0
2	EDO	A	213	4/4	0.93	0.28	69,71,72,75	0
2	EDO	A	207	4/4	0.93	0.33	40,42,51,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	206	4/4	0.93	0.21	82,84,84,85	0
2	EDO	B	207	4/4	0.94	0.45	61,62,65,65	0
2	EDO	A	208	4/4	0.94	0.19	62,65,66,68	0
2	EDO	D	206	4/4	0.98	0.20	47,48,48,62	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.