



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:54 am BST

PDB ID : 3SF5  
Title : Crystal Structure of Helicobacter pylori Urease Accessory Protein UreF/H complex  
Authors : Fong, Y.H.; Chen, Y.W.; Wong, K.B.  
Deposited on : 2011-06-12  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

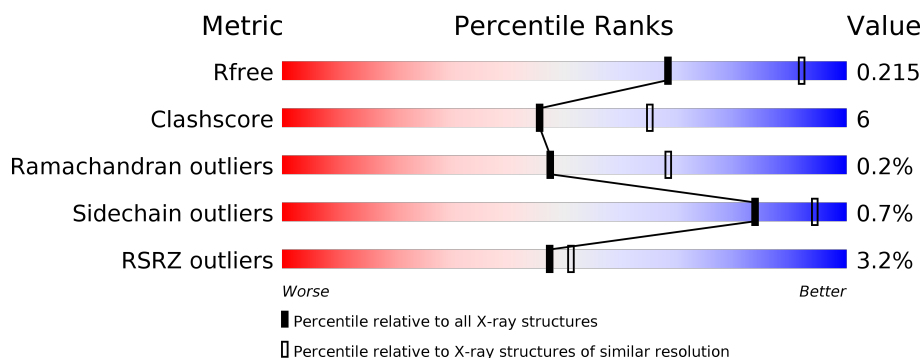
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>
1	C	254	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
2	B	265	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>••</div> </div> </div>
2	D	265	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>

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
5	SO4	C	258	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8053 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.

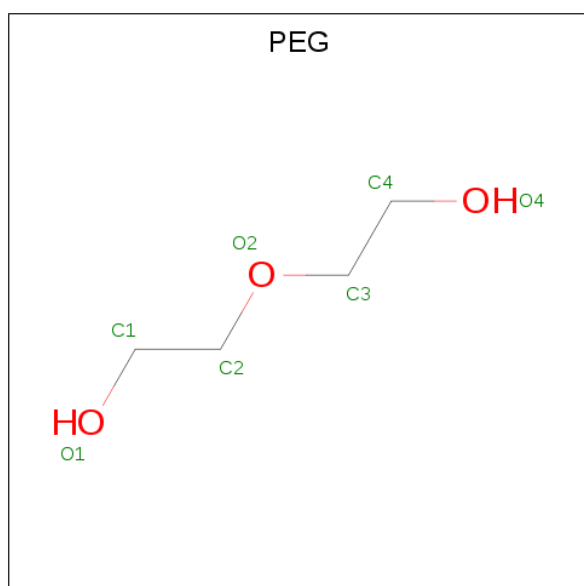
- Molecule 1 is a protein called Urease accessory protein ureF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1822	1159	300	353	10			
1	C	230	Total	C	N	O	S	0	0	0
			1830	1163	302	355	10			

- Molecule 2 is a protein called Urease accessory protein ureH.

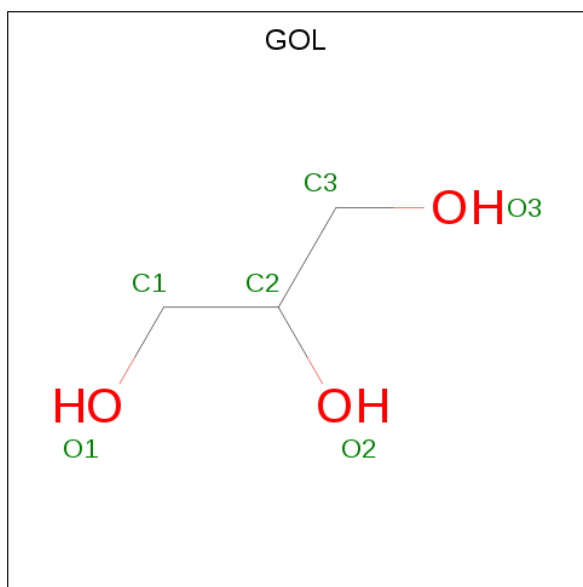
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2050	1299	349	389	13			
2	D	260	Total	C	N	O	S	0	0	0
			2044	1296	347	388	13			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

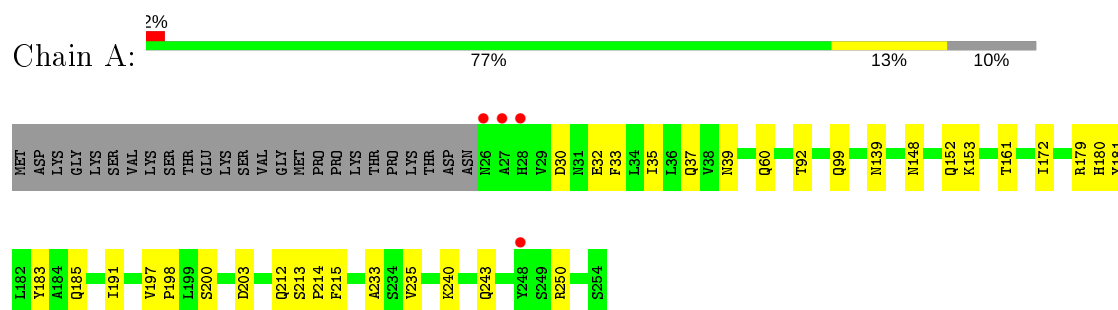
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		
6	B	53	Total	O	0	0
			53	53		
6	C	64	Total	O	0	0
			64	64		
6	D	30	Total	O	0	0
			30	30		

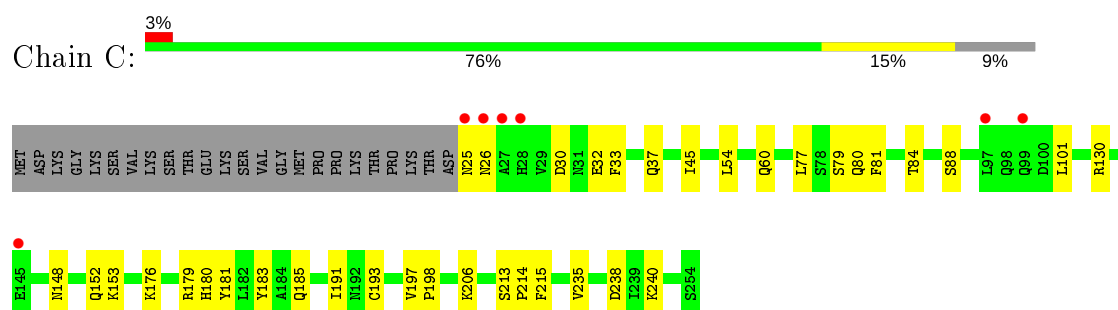
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

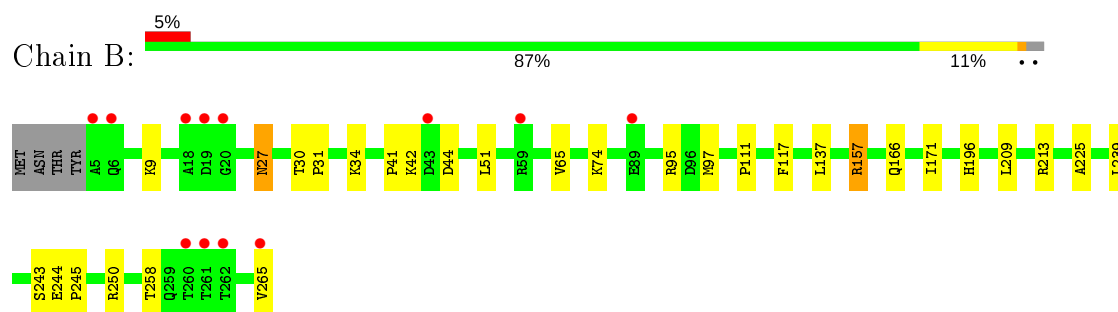
- Molecule 1: Urease accessory protein ureF



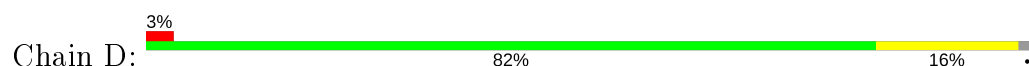
- Molecule 1: Urease accessory protein ureF

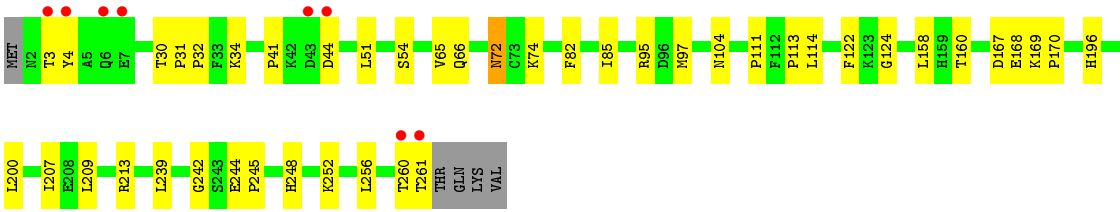


- Molecule 2: Urease accessory protein ureH



- Molecule 2: Urease accessory protein ureH







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.65Å 70.73Å 205.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.83 – 2.50 35.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (35.83-2.50) 99.1 (35.83-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.72 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4 _486)	Depositor
R, $R_{free}$	0.173 , 0.217 0.170 , 0.215	Depositor DCC
$R_{free}$ test set	1820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: GOL, PEG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.23	0/1852	0.38	0/2498
1	C	0.24	0/1860	0.38	0/2509
2	B	0.24	0/2089	0.43	0/2824
2	D	0.23	0/2084	0.41	0/2820
All	All	0.24	0/7885	0.40	0/10651

There are no bond length outliers.

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	1822	0	1834	27	0
1	C	1830	0	1840	28	0
2	B	2050	0	2057	25	0
2	D	2044	0	2042	29	0
3	A	28	0	40	1	0
3	B	14	0	20	3	0
3	C	14	0	20	2	0
3	D	7	0	10	1	0
4	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	8	2	0
5	B	10	0	0	1	0
5	C	5	0	0	4	0
5	D	10	0	0	0	0
6	A	60	0	0	1	0
6	B	53	0	0	0	0
6	C	64	0	0	1	0
6	D	30	0	0	0	0
All	All	8053	0	7879	100	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 6.

All (100) 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)
2:B:243:SER:H	3:B:268:PEG:H12	1.34	0.93
2:D:85:ILE:HD11	2:D:114:LEU:HD22	1.68	0.76
2:D:30:THR:HG23	2:D:31:PRO:HD2	1.71	0.72
2:B:34:LYS:HD3	2:B:51:LEU:HD11	1.75	0.68
1:A:39:ASN:OD1	3:A:258:PEG:H42	1.93	0.68
1:C:25:ASN:O	1:C:26:ASN:HB2	1.93	0.68
2:B:30:THR:HG23	2:B:31:PRO:HD2	1.79	0.64
2:D:34:LYS:HD3	2:D:51:LEU:HD11	1.80	0.64
1:C:213:SER:HB3	1:C:214:PRO:HD3	1.80	0.63
2:D:44:ASP:OD2	2:D:74:LYS:HD2	1.97	0.63
1:A:179:ARG:HG3	1:C:33:PHE:CE1	2.33	0.62
2:B:65:VAL:HB	2:B:97:MET:HG2	1.80	0.61
2:D:65:VAL:HB	2:D:97:MET:HG2	1.82	0.61
1:A:180:HIS:HE1	5:C:258:SO4:O2	1.84	0.60
1:A:37:GLN:HA	1:C:183:TYR:OH	2.01	0.60
2:B:97:MET:HE3	2:B:111:PRO:HB3	1.85	0.58
1:A:183:TYR:OH	1:C:37:GLN:HA	2.04	0.58
1:A:235:VAL:HG11	2:B:239:LEU:HD21	1.86	0.58
2:B:209:LEU:HD21	2:B:213:ARG:CZ	2.34	0.57
1:A:213:SER:HB3	1:A:214:PRO:HD3	1.85	0.57
1:C:176:LYS:HE3	5:C:258:SO4:O4	2.05	0.56
2:D:3:THR:HG23	2:D:4:TYR:CD2	2.40	0.56
1:C:206:LYS:NZ	3:C:255:PEG:H41	2.21	0.56
1:C:206:LYS:HZ3	3:C:255:PEG:H41	1.71	0.55
1:A:180:HIS:HD2	6:A:290:HOH:O	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:MET:HE3	2:D:111:PRO:HB3	1.90	0.53
1:C:30:ASP:OD1	1:C:32:GLU:HG2	2.08	0.53
2:B:137:LEU:HD22	2:B:250:ARG:NH2	2.24	0.53
2:B:196:HIS:NE2	3:B:268:PEG:H41	2.24	0.53
2:D:209:LEU:HD21	2:D:213:ARG:CZ	2.40	0.52
1:C:60:GLN:OE1	1:C:240:LYS:HE3	2.09	0.52
1:A:180:HIS:CE1	5:C:258:SO4:O2	2.62	0.52
2:D:34:LYS:HB3	2:D:51:LEU:CD1	2.40	0.52
1:A:33:PHE:CE1	1:C:179:ARG:HG3	2.45	0.52
2:B:243:SER:N	3:B:268:PEG:H12	2.15	0.52
2:D:82:PHE:CD2	2:D:113:PRO:HB2	2.45	0.52
1:C:238:ASP:OD2	4:C:257:GOL:H12	2.10	0.51
2:B:265:VAL:HG13	2:B:265:VAL:O	2.11	0.51
1:A:92:THR:HG21	1:A:161:THR:HB	1.93	0.51
2:B:209:LEU:HD21	2:B:213:ARG:NH2	2.26	0.51
2:B:95:ARG:HD2	2:B:97:MET:HE3	1.93	0.50
2:D:252:LYS:O	2:D:256:LEU:HD23	2.10	0.50
2:B:9:LYS:H	2:B:30:THR:HB	1.78	0.48
1:C:180:HIS:HD2	6:C:300:HOH:O	1.96	0.48
2:D:196:HIS:NE2	3:D:268:PEG:H11	2.29	0.48
1:A:39:ASN:ND2	1:A:180:HIS:HB3	2.29	0.47
2:B:117:PHE:N	2:B:117:PHE:CD1	2.83	0.47
1:A:33:PHE:CZ	1:C:215:PHE:HB3	2.50	0.46
1:A:191:ILE:HD13	1:A:191:ILE:HA	1.75	0.46
2:B:34:LYS:HB3	2:B:51:LEU:CD1	2.45	0.46
2:D:85:ILE:HD13	2:D:122:PHE:HB2	1.98	0.46
2:D:95:ARG:HD2	2:D:97:MET:HE3	1.98	0.46
2:B:157:ARG:NH2	5:B:267:SO4:O4	2.43	0.45
2:D:200:LEU:C	2:D:200:LEU:HD23	2.36	0.45
2:D:242:GLY:O	2:D:245:PRO:HD2	2.16	0.45
1:C:181:TYR:O	1:C:185:GLN:HG2	2.16	0.45
1:C:79:SER:OG	1:C:80:GLN:N	2.49	0.45
2:D:167:ASP:O	2:D:168:GLU:HB2	2.17	0.45
2:D:34:LYS:HB3	2:D:51:LEU:HD11	1.99	0.45
1:C:197:VAL:N	1:C:198:PRO:HA	2.32	0.44
1:A:148:ASN:O	1:A:152:GLN:HG3	2.18	0.44
1:C:235:VAL:HG11	2:D:239:LEU:HD21	1.98	0.44
1:A:99:GLN:HB3	1:A:99:GLN:HE21	1.64	0.44
2:B:166:GLN:HB2	2:B:171:ILE:HD13	1.99	0.44
2:D:260:THR:HG22	2:D:261:THR:N	2.32	0.44
1:A:60:GLN:OE1	1:A:240:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HA	1:C:81:PHE:HB3	2.01	0.43
2:D:158:LEU:HD23	2:D:158:LEU:C	2.38	0.43
1:A:181:TYR:O	1:A:185:GLN:HG2	2.19	0.43
1:C:180:HIS:CE1	5:C:258:SO4:O4	2.71	0.43
1:A:233:ALA:HA	4:A:259:GOL:O3	2.18	0.43
2:D:209:LEU:HD21	2:D:213:ARG:NH2	2.34	0.43
1:A:197:VAL:N	1:A:198:PRO:HA	2.34	0.43
1:A:243:GLN:HG3	2:B:225:ALA:HB2	2.01	0.42
2:B:44:ASP:OD2	2:B:74:LYS:HD2	2.18	0.42
2:D:169:LYS:HA	2:D:170:PRO:HD3	1.90	0.42
2:B:34:LYS:HB3	2:B:51:LEU:HD11	2.01	0.42
1:C:84:THR:O	1:C:88:SER:HB3	2.20	0.42
1:C:80:GLN:OE1	4:C:257:GOL:H2	2.20	0.42
1:A:179:ARG:HG3	1:C:33:PHE:CZ	2.54	0.42
1:C:54:LEU:HD21	1:C:193:CYS:SG	2.60	0.42
2:D:32:PRO:HG3	2:D:54:SER:HB2	2.01	0.42
2:D:244:GLU:HB3	2:D:245:PRO:HD3	2.01	0.42
2:D:207:ILE:HD12	2:D:256:LEU:HB3	2.02	0.42
1:A:30:ASP:OD1	1:A:32:GLU:HG2	2.20	0.41
1:A:212:GLN:O	1:A:215:PHE:HB2	2.20	0.41
2:B:244:GLU:HB3	2:B:245:PRO:HD3	2.01	0.41
2:B:27:ASN:C	2:B:27:ASN:ND2	2.73	0.41
1:C:101:LEU:HD21	1:C:153:LYS:HD3	2.01	0.41
1:C:45:ILE:O	1:C:130:ARG:HD2	2.19	0.41
1:C:191:ILE:HA	1:C:191:ILE:HD13	1.85	0.41
1:C:148:ASN:O	1:C:152:GLN:HG3	2.21	0.41
2:D:72:ASN:HD22	2:D:104:ASN:HB3	1.85	0.41
1:A:153:LYS:HB3	1:A:153:LYS:HE2	1.97	0.41
1:A:35:ILE:HD13	1:A:172:ILE:HD13	2.02	0.41
2:D:124:GLY:O	2:D:160:THR:HA	2.21	0.41
1:A:200:SER:O	1:A:203:ASP:HB2	2.21	0.41
2:B:117:PHE:N	2:B:117:PHE:HD1	2.18	0.40
2:B:42:LYS:HE3	2:B:258:THR:CG2	2.52	0.40
2:D:248:HIS:CD2	2:D:252:LYS:HE3	2.56	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	227/254 (89%)	224 (99%)	3 (1%)	0	100	100
1	C	228/254 (90%)	222 (97%)	6 (3%)	0	100	100
2	B	259/265 (98%)	248 (96%)	10 (4%)	1 (0%)	34	54
2	D	258/265 (97%)	248 (96%)	9 (4%)	1 (0%)	34	54
All	All	972/1038 (94%)	942 (97%)	28 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	41	PRO
2	D	41	PRO

### 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	205/228 (90%)	203 (99%)	2 (1%)	76	90
1	C	206/228 (90%)	206 (100%)	0	100	100
2	B	230/234 (98%)	228 (99%)	2 (1%)	78	92
2	D	229/234 (98%)	227 (99%)	2 (1%)	78	92
All	All	870/924 (94%)	864 (99%)	6 (1%)	84	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	250	ARG
2	B	27	ASN
2	B	157	ARG
2	D	66	GLN
2	D	72	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	99	GLN
1	A	125	GLN
1	A	148	ASN
1	A	180	HIS
1	A	185	GLN
1	A	217	GLN
1	A	229	HIS
1	A	237	ASN
2	B	27	ASN
2	B	125	ASN
2	B	259	GLN
1	C	98	GLN
1	C	99	GLN
1	C	136	GLN
1	C	148	ASN
1	C	180	HIS
1	C	192	ASN
1	C	217	GLN
2	D	2	ASN
2	D	72	ASN
2	D	80	GLN
2	D	104	ASN
2	D	186	ASN
2	D	259	GLN

### 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 carbohydrates 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	$\# Z  > 2$
5	SO4	D	267	-	4,4,4	0.14	0	6,6,6	0.07	0
3	PEG	A	255	-	6,6,6	0.64	0	5,5,5	1.45	0
3	PEG	C	256	-	6,6,6	0.64	0	5,5,5	1.39	0
4	GOL	A	259	-	5,5,5	0.34	0	5,5,5	0.36	0
3	PEG	A	256	-	6,6,6	0.61	0	5,5,5	1.48	0
4	GOL	C	257	-	5,5,5	0.37	0	5,5,5	0.27	0
3	PEG	D	268	-	6,6,6	0.65	0	5,5,5	1.41	0
3	PEG	A	257	-	6,6,6	0.63	0	5,5,5	1.40	0
3	PEG	A	258	-	6,6,6	0.63	0	5,5,5	1.41	0
5	SO4	B	266	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	D	266	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	267	-	4,4,4	0.14	0	6,6,6	0.07	0
3	PEG	B	268	-	6,6,6	0.62	0	5,5,5	1.51	0
3	PEG	B	269	-	6,6,6	0.64	0	5,5,5	1.37	0
5	SO4	C	258	-	4,4,4	0.14	0	6,6,6	0.09	0
3	PEG	C	255	-	6,6,6	0.64	0	5,5,5	1.29	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	PEG	A	255	-	-	1/4/4/4	-
3	PEG	C	256	-	-	1/4/4/4	-
4	GOL	A	259	-	-	4/4/4/4	-
3	PEG	A	256	-	-	3/4/4/4	-
4	GOL	C	257	-	-	2/4/4/4	-
3	PEG	D	268	-	-	1/4/4/4	-
3	PEG	A	257	-	-	0/4/4/4	-
3	PEG	A	258	-	-	1/4/4/4	-
3	PEG	B	268	-	-	2/4/4/4	-
3	PEG	B	269	-	-	1/4/4/4	-
3	PEG	C	255	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	259	GOL	C1-C2-C3-O3
4	C	257	GOL	O1-C1-C2-C3
4	C	257	GOL	O1-C1-C2-O2
3	C	256	PEG	O2-C3-C4-O4
4	A	259	GOL	O1-C1-C2-C3
3	A	258	PEG	O2-C3-C4-O4
4	A	259	GOL	O2-C2-C3-O3
4	A	259	GOL	O1-C1-C2-O2
3	A	255	PEG	O2-C3-C4-O4
3	C	255	PEG	O1-C1-C2-O2
3	A	256	PEG	C1-C2-O2-C3
3	B	269	PEG	C1-C2-O2-C3
3	A	256	PEG	C4-C3-O2-C2
3	A	256	PEG	O1-C1-C2-O2
3	D	268	PEG	C1-C2-O2-C3
3	B	268	PEG	O1-C1-C2-O2
3	C	255	PEG	O2-C3-C4-O4
3	B	268	PEG	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	259	GOL	1	0
4	C	257	GOL	2	0
3	D	268	PEG	1	0
3	A	258	PEG	1	0
5	B	267	SO4	1	0
3	B	268	PEG	3	0
5	C	258	SO4	4	0
3	C	255	PEG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	229/254 (90%)	-0.25	4 (1%) 70 72	17, 25, 43, 95	0
1	C	230/254 (90%)	-0.14	7 (3%) 50 53	16, 25, 45, 85	0
2	B	261/265 (98%)	-0.06	12 (4%) 32 34	17, 30, 59, 83	0
2	D	260/265 (98%)	-0.02	8 (3%) 49 52	18, 32, 62, 110	0
All	All	980/1038 (94%)	-0.12	31 (3%) 47 51	16, 28, 54, 110	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	9.2
2	D	261	THR	8.7
2	D	4	TYR	5.4
1	C	25	ASN	5.2
2	B	18	ALA	4.8
1	A	26	ASN	4.8
2	B	5	ALA	4.4
2	D	43	ASP	3.4
2	D	3	THR	3.3
2	B	261	THR	3.1
2	D	44	ASP	3.1
2	D	260	THR	2.8
1	C	27	ALA	2.8
2	B	6	GLN	2.8
2	B	262	THR	2.7
2	D	6	GLN	2.6
2	B	20	GLY	2.6
1	A	28	HIS	2.6
1	C	26	ASN	2.6
2	B	19	ASP	2.5
1	A	248	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	265	VAL	2.5
1	C	97	LEU	2.4
2	D	7	GLU	2.4
1	C	28	HIS	2.3
1	C	99	GLN	2.3
2	B	43	ASP	2.3
2	B	260	THR	2.2
2	B	59	ARG	2.2
2	B	89	GLU	2.1
1	C	145	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	A	258	7/7	0.81	0.27	29,35,47,64	0
3	PEG	A	257	7/7	0.85	0.28	39,53,60,63	0
3	PEG	B	269	7/7	0.88	0.21	41,47,55,59	0
3	PEG	D	268	7/7	0.89	0.12	41,46,55,56	0
3	PEG	B	268	7/7	0.89	0.20	36,42,50,50	0
3	PEG	A	256	7/7	0.89	0.21	42,45,50,54	0
3	PEG	C	256	7/7	0.90	0.16	39,45,57,61	0
5	SO4	C	258	5/5	0.91	0.19	54,65,85,88	0
3	PEG	C	255	7/7	0.92	0.17	21,39,45,65	0
4	GOL	C	257	6/6	0.93	0.23	28,29,43,46	0
4	GOL	A	259	6/6	0.94	0.18	25,32,35,38	0
3	PEG	A	255	7/7	0.94	0.19	38,43,51,57	0
5	SO4	D	267	5/5	0.98	0.20	41,47,53,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	D	266	5/5	0.99	0.11	28,31,42,46	0
5	SO4	B	267	5/5	0.99	0.12	36,39,43,53	0
5	SO4	B	266	5/5	0.99	0.15	27,41,44,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.