Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 05:20 AM EDT

PDB ID	:	6BI8
Title	:	X-ray structure of MERS coronavirus papain-like protease in complex with human ISG15
Authors	:	Clasman, J.C.; Mesecar, A.D.
Deposited on	:	2017-11-01
Resolution	:	2.29 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:

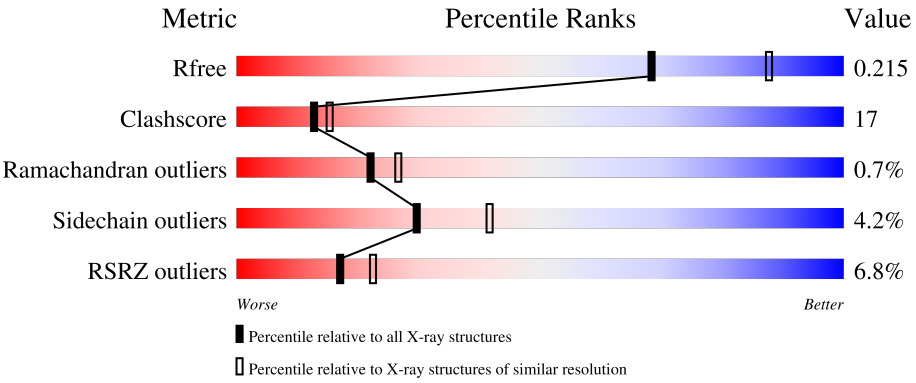
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	259	81% 19%
1	B	259	88% 12%
2	C	156	19% 56% 35% 7% •
2	D	156	17% 52% 38% 8% •

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
5	GOL	B	1906	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7018 atoms, of which 125 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 ORF1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	3	0
			2045	1305	352	369	19			
1	B	259	Total	C	N	O	S	0	2	0
			2036	1301	350	366	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1543	ASN	-	expression tag	UNP K4LC41
B	1543	ASN	-	expression tag	UNP K4LC41

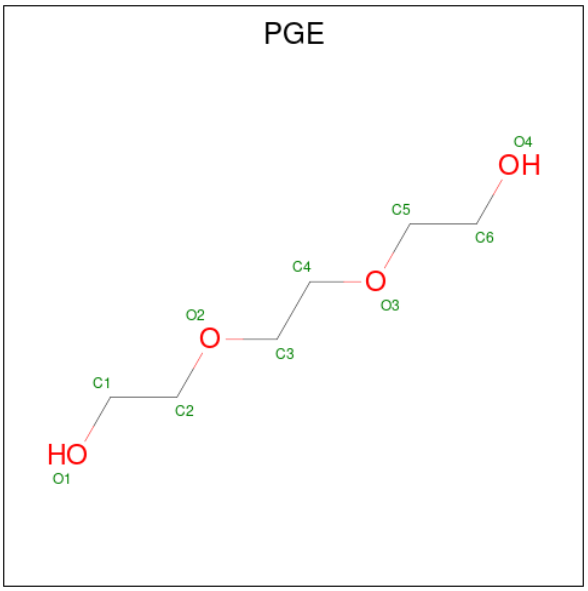
- Molecule 2 is a protein called Ubiquitin-like protein ISG15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	153	Total	C	N	O	S	0	0	0
			1153	729	200	221	3			
2	D	153	Total	C	N	O	S	0	0	0
			1159	732	203	221	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	78	SER	CYS	engineered mutation	UNP P05161
D	78	SER	CYS	engineered mutation	UNP P05161

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

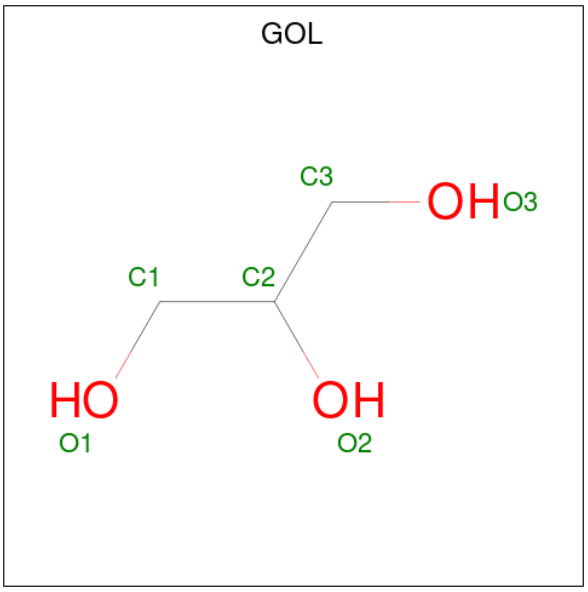


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 24 6 14 4	0	0
3	B	1	Total C H O 24 6 14 4	0	0
3	B	1	Total C H O 24 6 14 4	0	0
3	C	1	Total C H O 24 6 14 4	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

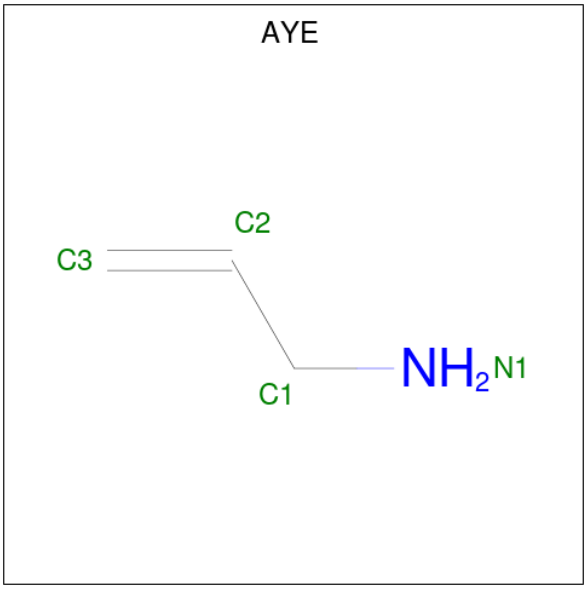
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



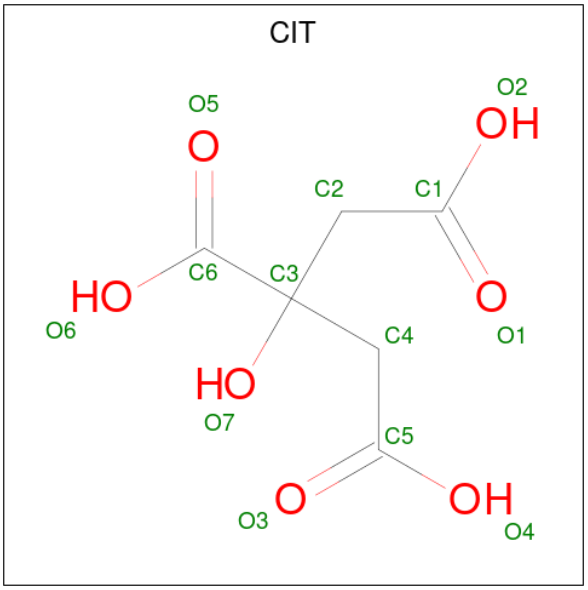
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0

- Molecule 6 is prop-2-en-1-amine (three-letter code: AYE) (formula: C_3H_7N).



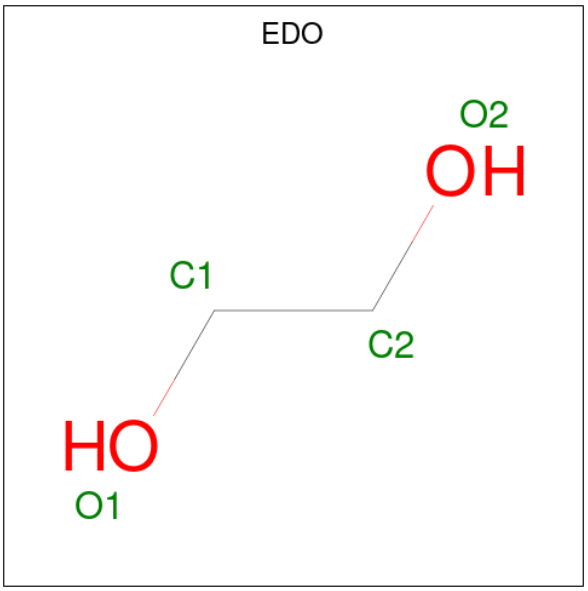
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	N	0	0
			10	3	6	1		
6	B	1	Total	C	H	N	0	0
			10	3	6	1		

- Molecule 7 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			10	2	6	2		
8	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 9 is water.

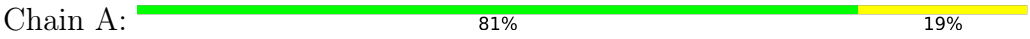
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	156	Total	O	0	4
			160	160		
9	B	163	Total	O	0	1
			164	164		
9	C	39	Total	O	0	0
			39	39		
9	D	36	Total	O	0	0
			36	36		

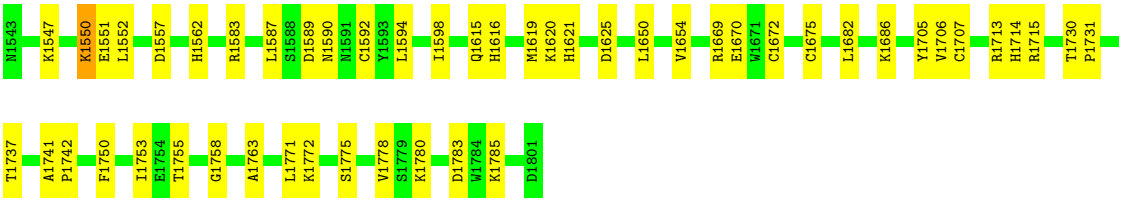
3 Residue-property plots (i)

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: ORF1a

Chain A:



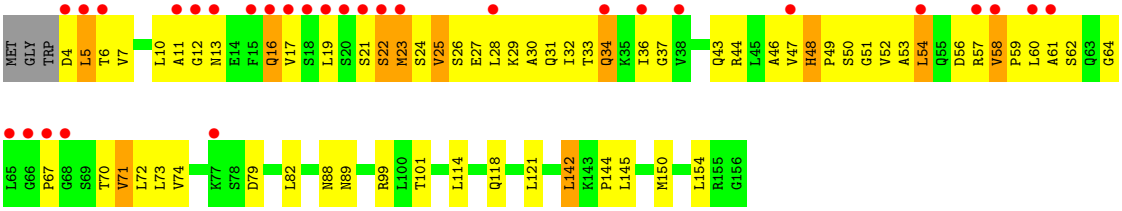


• Molecule 1: ORF1a

Chain B:

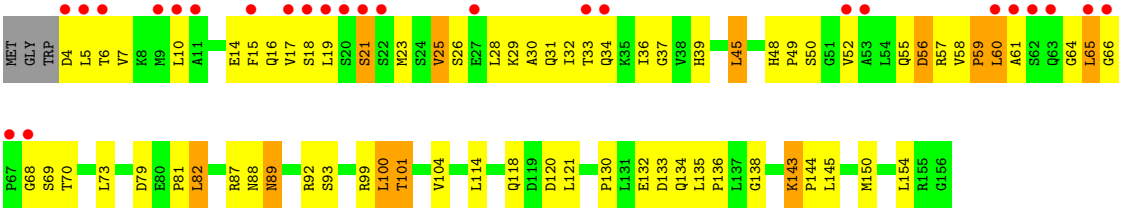
• Molecule 2: Ubiquitin-like protein ISG15

Chain C:



• Molecule 2: Ubiquitin-like protein ISG15

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	148.03Å 148.03Å 134.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.73 – 2.29 42.73 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.73-2.29) 98.3 (42.73-2.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.76 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.172 , 0.215 0.173 , 0.215	Depositor DCC
R_{free} test set	2006 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7018	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, AYE, ZN, GOL, EDO, CIT

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	0.47	0/2091	0.56	0/2832
1	B	0.47	0/2085	0.56	0/2824
2	C	0.33	0/1171	0.53	0/1588
2	D	0.33	0/1177	0.48	0/1596
All	All	0.42	0/6524	0.54	0/8840

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

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	2045	0	2043	40	0
1	B	2036	0	2040	28	0
2	C	1153	0	1165	74	0
2	D	1159	0	1161	86	0
3	A	10	14	14	0	0
3	B	20	28	28	1	0
3	C	10	14	14	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	16	16	1	0
5	B	18	24	24	5	0
6	A	4	6	4	1	0
6	B	4	6	4	0	0
7	B	13	5	5	0	0
8	B	8	12	12	0	0
9	A	160	0	0	5	0
9	B	164	0	0	2	0
9	C	39	0	0	0	0
9	D	36	0	0	0	0
All	All	6893	125	6530	216	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 17.

All (216) 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:D:104:VAL:HB	2:D:133:ASP:HA	1.38	1.05
2:C:7:VAL:HG12	2:C:71:VAL:HG12	1.47	0.96
2:C:11:ALA:HB3	2:C:13:ASN:H	1.32	0.93
2:C:61:ALA:HA	2:C:62:SER:HB3	1.48	0.91
2:D:19:LEU:HD11	2:D:31:GLN:HG3	1.55	0.89
2:C:23:MET:HB3	2:C:59:PRO:HB2	1.57	0.86
2:C:11:ALA:N	2:C:12:GLY:HA2	1.93	0.81
2:C:5:LEU:HB3	2:C:17:VAL:HG12	1.63	0.80
1:A:1550:LYS:HE3	2:C:34:GLN:HE22	1.46	0.79
2:D:64:GLY:HA3	2:D:65:LEU:HD22	1.66	0.77
2:D:65:LEU:H	2:D:69:SER:HB2	1.48	0.75
2:C:23:MET:O	2:C:59:PRO:HB3	1.87	0.75
2:C:11:ALA:HB3	2:C:13:ASN:N	2.00	0.74
2:C:61:ALA:HB2	2:C:64:GLY:H	1.52	0.74
2:D:57:ARG:HH11	2:D:58:VAL:HA	1.52	0.74
2:C:5:LEU:HD22	2:C:6:THR:H	1.52	0.74
2:C:21:SER:O	2:C:23:MET:N	2.21	0.74
1:B:1707:CYS:HB2	1:B:1713:ARG:HB2	1.71	0.71
2:D:29:LYS:O	2:D:33:THR:N	2.22	0.71
2:D:118:GLN:HB3	2:D:121:LEU:HG	1.72	0.71
2:D:5:LEU:CD1	2:D:66:GLY:HA3	2.20	0.71
1:A:1550:LYS:HE3	2:C:34:GLN:NE2	2.06	0.71
1:B:1669:ARG:NH2	9:B:2001:HOH:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:LEU:HG	2:D:65:LEU:HD13	1.72	0.70
2:D:45:LEU:CD1	2:D:73:LEU:HD23	2.22	0.70
1:A:1682:LEU:HD21	1:A:1686:LYS:HB2	1.72	0.70
2:C:89:ASN:H	2:C:150:MET:HE2	1.57	0.70
1:A:1707:CYS:HB2	1:A:1713:ARG:HB2	1.73	0.69
1:B:1715:ARG:HH21	5:B:1906:GOL:H11	1.58	0.69
2:C:23:MET:HB3	2:C:59:PRO:CB	2.21	0.69
1:A:1594:LEU:O	1:A:1598:ILE:HG12	1.93	0.69
2:C:17:VAL:HG22	2:C:19:LEU:HG	1.75	0.68
2:D:57:ARG:NH1	2:D:59:PRO:HD2	2.09	0.68
2:C:47:VAL:HA	2:C:71:VAL:HG23	1.76	0.68
1:A:1706:VAL:CG2	2:C:145:LEU:HB3	2.24	0.68
2:D:104:VAL:CB	2:D:133:ASP:HA	2.20	0.68
2:D:114:LEU:O	2:D:114:LEU:HD23	1.93	0.67
2:C:32:ILE:O	2:C:36:ILE:HG22	1.94	0.67
1:B:1550:LYS:HZ1	1:B:1555:PRO:HB3	1.60	0.67
2:C:88:ASN:HB2	2:C:150:MET:HE1	1.77	0.66
2:D:57:ARG:HD3	2:D:58:VAL:H	1.60	0.66
2:D:66:GLY:HA2	2:D:68:GLY:N	2.11	0.66
2:D:6:THR:HG23	2:D:70:THR:HG23	1.76	0.66
2:C:118:GLN:HB2	2:C:121:LEU:HG	1.78	0.65
1:B:1715:ARG:HH21	5:B:1906:GOL:C1	2.10	0.64
1:B:1550:LYS:NZ	1:B:1555:PRO:HB3	2.12	0.64
2:D:25:VAL:O	2:D:28:LEU:HB3	1.98	0.63
2:D:26:SER:HA	2:D:29:LYS:HG3	1.80	0.63
2:D:4:ASP:HA	2:D:17:VAL:O	1.98	0.63
2:D:50:SER:HB2	2:D:52:VAL:HG23	1.78	0.63
2:D:118:GLN:HG2	2:D:120:ASP:OD1	1.99	0.63
1:A:1730:THR:HG22	9:A:2050:HOH:O	1.99	0.63
2:D:50:SER:CB	2:D:52:VAL:HG23	2.29	0.63
2:D:82:LEU:HD21	2:D:100:LEU:HD13	1.81	0.63
2:C:6:THR:HA	2:C:16:GLN:HA	1.81	0.62
1:A:1682:LEU:HD21	1:A:1686:LYS:CB	2.28	0.62
2:D:45:LEU:HD13	2:D:73:LEU:HD23	1.82	0.62
2:C:4:ASP:OD2	2:C:16:GLN:HG3	2.01	0.61
2:D:7:VAL:HG21	2:D:15:PHE:CZ	2.35	0.61
1:A:1625:ASP:HB2	3:B:1902:PGE:H4	1.83	0.61
2:C:53:ALA:O	2:C:54:LEU:HB2	2.01	0.60
2:C:61:ALA:CB	2:C:64:GLY:H	2.15	0.59
1:A:1669:ARG:NH1	9:A:2012:HOH:O	2.36	0.59
2:C:58:VAL:HG12	2:C:59:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1550:LYS:HE2	2:D:34:GLN:HG2	1.86	0.58
2:D:6:THR:HA	2:D:16:GLN:HA	1.86	0.58
2:D:5:LEU:HD11	2:D:66:GLY:HA3	1.85	0.57
2:C:61:ALA:HB2	2:C:64:GLY:O	2.05	0.57
1:B:1615:GLN:O	1:B:1619[B]:MET:HG3	2.03	0.57
2:D:60:LEU:HG	2:D:64:GLY:HA2	1.86	0.57
1:A:1672:CYS:HB3	1:A:1675:CYS:HB2	1.85	0.57
1:B:1636:TYR:CD1	1:B:1657:LYS:HE3	2.40	0.57
1:A:1620:LYS:HG3	1:B:1552:LEU:HD21	1.87	0.56
2:D:5:LEU:O	2:D:17:VAL:N	2.37	0.56
2:D:57:ARG:NH1	2:D:58:VAL:HA	2.18	0.56
2:C:44:ARG:HB2	2:C:74:VAL:CG2	2.35	0.56
2:D:65:LEU:H	2:D:69:SER:CB	2.17	0.56
1:B:1550:LYS:HE2	2:D:34:GLN:CG	2.36	0.56
2:D:5:LEU:HD12	2:D:66:GLY:HA3	1.86	0.56
2:C:5:LEU:HB3	2:C:17:VAL:CG1	2.35	0.56
2:D:60:LEU:CG	2:D:65:LEU:HD13	2.35	0.56
2:C:88:ASN:HB2	2:C:150:MET:CE	2.36	0.55
2:C:89:ASN:H	2:C:150:MET:CE	2.19	0.55
1:B:1670:GLU:OE2	5:B:1906:GOL:O1	2.26	0.54
1:A:1552:LEU:HD21	1:B:1620:LYS:HG2	1.89	0.54
2:C:5:LEU:CD2	2:C:6:THR:H	2.18	0.54
1:B:1669:ARG:O	1:B:1715:ARG:HA	2.08	0.54
1:A:1706:VAL:HG21	2:C:145:LEU:HB3	1.89	0.53
2:C:26:SER:O	2:C:29:LYS:HB2	2.08	0.53
2:C:29:LYS:O	2:C:33:THR:N	2.33	0.53
2:C:34:GLN:NE2	2:C:34:GLN:O	2.42	0.53
2:D:64:GLY:CA	2:D:65:LEU:HD22	2.36	0.53
1:A:1686:LYS:HG2	5:A:1904:GOL:H11	1.90	0.52
2:C:61:ALA:HA	2:C:62:SER:CB	2.21	0.52
1:A:1669:ARG:O	1:A:1715:ARG:HA	2.09	0.52
2:D:17:VAL:HG21	2:D:28:LEU:HD13	1.91	0.52
1:B:1564:PHE:CE1	1:B:1632:LEU:HD13	2.45	0.52
2:C:29:LYS:HD2	2:C:43:GLN:OE1	2.09	0.52
2:D:88:ASN:HA	2:D:150:MET:HB3	1.92	0.52
1:B:1731:PRO:CG	2:D:154:LEU:HD11	2.39	0.52
1:A:1771:LEU:HD23	1:A:1780:LYS:HG2	1.92	0.51
1:B:1611:ILE:HD12	1:B:1657:LYS:HD3	1.92	0.51
2:D:55:GLN:HB2	2:D:58:VAL:HB	1.93	0.51
2:D:18:SER:O	2:D:19:LEU:HD23	2.10	0.51
2:C:27:GLU:O	2:C:31:GLN:N	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ALA:HA	2:C:33:THR:OG1	2.10	0.51
1:A:1753:ILE:HG22	1:A:1755:THR:H	1.76	0.50
5:B:1905:GOL:H12	2:D:130:PRO:HD2	1.92	0.50
1:A:1615:GLN:O	1:A:1619[A]:MET:HG3	2.11	0.50
1:B:1715:ARG:HE	5:B:1906:GOL:C1	2.24	0.50
2:C:28:LEU:O	2:C:32:ILE:HG13	2.12	0.50
2:D:143:LYS:HB3	2:D:144:PRO:HD2	1.94	0.50
2:C:25:VAL:O	2:C:28:LEU:HB3	2.11	0.50
2:C:5:LEU:O	2:C:16:GLN:HB2	2.12	0.50
2:C:7:VAL:HG12	2:C:71:VAL:CG1	2.31	0.50
2:C:79:ASP:OD1	2:C:79:ASP:N	2.45	0.50
2:C:25:VAL:O	2:C:29:LYS:HG2	2.11	0.50
2:D:28:LEU:O	2:D:32:ILE:HG13	2.12	0.50
2:D:60:LEU:HG	2:D:64:GLY:CA	2.42	0.50
1:A:1731:PRO:CG	2:C:154:LEU:HD11	2.42	0.49
1:A:1730:THR:OG1	1:A:1731:PRO:HD2	2.12	0.49
2:D:64:GLY:HA3	2:D:65:LEU:CD2	2.39	0.49
1:A:1771:LEU:CD2	1:A:1780:LYS:HG2	2.43	0.49
2:C:79:ASP:O	2:C:99:ARG:NH1	2.43	0.49
2:C:114:LEU:O	2:C:114:LEU:HD12	2.13	0.49
1:B:1730:THR:OG1	1:B:1731:PRO:HD2	2.12	0.49
2:D:17:VAL:HG21	2:D:28:LEU:CD1	2.43	0.49
2:D:144:PRO:O	2:D:145:LEU:HB2	2.13	0.49
2:D:50:SER:OG	2:D:52:VAL:HG23	2.13	0.49
1:B:1730:THR:HG22	9:B:2080:HOH:O	2.12	0.48
2:C:17:VAL:HG13	2:C:17:VAL:O	2.13	0.48
2:D:21:SER:O	2:D:23:MET:HG3	2.13	0.48
1:A:1583:ARG:NH2	1:A:1621:HIS:O	2.46	0.48
2:C:89:ASN:N	2:C:150:MET:HE2	2.27	0.48
2:C:5:LEU:HD22	2:C:6:THR:N	2.22	0.48
2:D:57:ARG:CD	2:D:58:VAL:H	2.26	0.48
2:C:5:LEU:CB	2:C:17:VAL:HG12	2.40	0.48
2:D:17:VAL:HG12	2:D:19:LEU:HB2	1.95	0.48
1:B:1543:ASN:O	1:B:1547:LYS:HG3	2.13	0.47
2:D:64:GLY:HA3	2:D:65:LEU:CB	2.44	0.47
2:D:17:VAL:CG1	2:D:19:LEU:HB2	2.45	0.47
1:B:1763:ALA:HA	1:B:1771:LEU:O	2.14	0.47
2:C:50:SER:O	2:C:52:VAL:N	2.47	0.47
1:A:1713:ARG:NH2	9:A:2003:HOH:O	2.27	0.47
2:C:5:LEU:HD22	2:C:6:THR:O	2.15	0.47
2:D:50:SER:HB2	2:D:52:VAL:CG2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1672:CYS:HB3	1:B:1675:CYS:HB2	1.97	0.47
2:D:17:VAL:HG13	2:D:19:LEU:HG	1.96	0.47
1:A:1705:TYR:OH	1:A:1713:ARG:HD3	2.16	0.46
2:C:44:ARG:HB2	2:C:74:VAL:HG22	1.97	0.46
2:D:79:ASP:OD1	2:D:101:THR:HB	2.15	0.46
2:C:44:ARG:HB2	2:C:74:VAL:HG23	1.97	0.46
2:D:33:THR:O	2:D:37:GLY:HA2	2.16	0.46
2:C:33:THR:O	2:C:37:GLY:N	2.50	0.45
2:C:46:ALA:O	2:C:71:VAL:HG22	2.16	0.45
2:D:87:ARG:HD3	2:D:93:SER:OG	2.16	0.45
2:D:82:LEU:CD2	2:D:100:LEU:HD13	2.47	0.45
2:C:22:SER:O	2:C:23:MET:HB2	2.17	0.45
2:C:144:PRO:O	2:C:145:LEU:HB2	2.17	0.45
2:D:56:ASP:O	2:D:58:VAL:HG23	2.16	0.45
2:C:70:THR:HG22	2:C:71:VAL:N	2.32	0.45
2:D:100:LEU:HG	2:D:138:GLY:HA2	1.97	0.44
2:D:30:ALA:HA	2:D:33:THR:HB	1.99	0.44
1:A:1547:LYS:O	1:A:1551:GLU:HG3	2.16	0.44
1:A:1731:PRO:HG2	2:C:154:LEU:HD11	2.00	0.44
1:B:1589:ASP:O	1:B:1590:ASN:HB2	2.18	0.44
1:A:1772:LYS:O	1:A:1778:VAL:HA	2.18	0.44
1:A:1592:CYS:HB3	6:A:1905:AYE:H3A	1.92	0.43
2:D:65:LEU:HD13	2:D:65:LEU:HA	1.80	0.43
1:A:1750:PHE:CZ	1:A:1758:GLY:HA3	2.54	0.43
2:D:5:LEU:HD11	2:D:66:GLY:H	1.83	0.43
1:A:1741:ALA:HA	1:A:1742:PRO:HD3	1.93	0.43
2:D:60:LEU:HD23	2:D:65:LEU:CD1	2.48	0.43
1:A:1587:LEU:HB2	1:A:1775:SER:HB3	2.00	0.43
2:C:72:LEU:HG	2:C:73:LEU:N	2.33	0.43
2:C:47:VAL:HG13	2:C:54:LEU:HD11	2.00	0.42
2:D:58:VAL:HG13	2:D:61:ALA:HB3	2.00	0.42
2:D:81:PRO:HG3	2:D:99:ARG:NH1	2.34	0.42
2:C:59:PRO:HA	2:C:60:LEU:HA	1.64	0.42
2:C:10:LEU:HD12	2:C:10:LEU:N	2.34	0.42
2:D:57:ARG:CG	2:D:58:VAL:H	2.32	0.42
1:A:1785:LYS:NZ	9:A:2023:HOH:O	2.52	0.42
2:C:48:HIS:HA	2:C:49:PRO:HA	1.74	0.42
2:C:61:ALA:CA	2:C:62:SER:HB3	2.35	0.42
2:D:36:ILE:O	2:D:36:ILE:HG13	2.20	0.42
2:D:132:GLU:HB3	2:D:134:GLN:NE2	2.35	0.42
1:B:1561:LEU:HD12	1:B:1561:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:ASN:HD21	2:D:92:ARG:HG2	1.83	0.42
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.20	0.42
1:A:1670:GLU:HA	1:A:1714:HIS:O	2.20	0.42
1:B:1564:PHE:CZ	1:B:1632:LEU:HD13	2.55	0.42
2:D:82:LEU:HD21	2:D:100:LEU:CD1	2.50	0.41
1:A:1737:THR:HG22	1:A:1783:ASP:CG	2.41	0.41
1:A:1589:ASP:O	1:A:1590:ASN:HB2	2.20	0.41
1:A:1616:HIS:CD2	1:B:1552:LEU:HD11	2.55	0.41
2:C:4:ASP:N	2:C:67:PRO:HG3	2.36	0.41
2:D:14:GLU:OE1	2:D:14:GLU:N	2.50	0.41
2:C:5:LEU:CD2	2:C:6:THR:N	2.82	0.41
2:C:142:LEU:HD12	2:C:142:LEU:HA	1.85	0.41
2:D:5:LEU:HD11	2:D:66:GLY:CA	2.48	0.41
2:D:30:ALA:HA	2:D:33:THR:CB	2.50	0.41
2:D:135:LEU:HD23	2:D:135:LEU:HA	1.90	0.41
1:A:1562[B]:HIS:ND1	9:A:2013:HOH:O	2.37	0.40
2:D:30:ALA:O	2:D:33:THR:HB	2.20	0.40
1:A:1763:ALA:HA	1:A:1771:LEU:O	2.21	0.40
2:D:89:ASN:OD1	2:D:89:ASN:N	2.50	0.40
1:B:1670:GLU:HA	1:B:1714:HIS:O	2.21	0.40
2:C:29:LYS:O	2:C:32:ILE:HB	2.21	0.40
2:D:134:GLN:H	2:D:134:GLN:CD	2.25	0.40
2:C:60:LEU:O	2:C:62:SER:HB3	2.22	0.40
2:D:39:HIS:CG	2:D:136:PRO:HG3	2.56	0.40
2:D:64:GLY:HA3	2:D:65:LEU:CG	2.52	0.40
2:D:30:ALA:HA	2:D:33:THR:OG1	2.22	0.40
2:D:45:LEU:HD12	2:D:45:LEU:HA	1.71	0.40
2:D:48:HIS:HA	2:D:49:PRO:HA	1.86	0.40
2:D:79:ASP:OD1	2:D:99:ARG:HB3	2.21	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	260/259 (100%)	255 (98%)	5 (2%)	0	100 100
1	B	259/259 (100%)	254 (98%)	5 (2%)	0	100 100
2	C	151/156 (97%)	132 (87%)	15 (10%)	4 (3%)	5 4
2	D	151/156 (97%)	138 (91%)	11 (7%)	2 (1%)	12 12
All	All	821/830 (99%)	779 (95%)	36 (4%)	6 (1%)	22 26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	22	SER
2	C	51	GLY
2	C	57	ARG
2	D	21	SER
2	D	59	PRO
2	C	54	LEU

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	225/222 (101%)	223 (99%)	2 (1%)	78 89
1	B	224/222 (101%)	221 (99%)	3 (1%)	69 82
2	C	128/135 (95%)	115 (90%)	13 (10%)	7 8
2	D	126/135 (93%)	115 (91%)	11 (9%)	10 12
All	All	703/714 (98%)	674 (96%)	29 (4%)	30 43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1550	LYS
1	A	1557	ASP
1	B	1551	GLU
1	B	1557	ASP
1	B	1735	LEU

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Mol	Chain	Res	Type
2	C	5	LEU
2	C	16	GLN
2	C	23	MET
2	C	24	SER
2	C	25	VAL
2	C	34	GLN
2	C	48	HIS
2	C	56	ASP
2	C	58	VAL
2	C	71	VAL
2	C	82	LEU
2	C	101	THR
2	C	142	LEU
2	D	10	LEU
2	D	25	VAL
2	D	45	LEU
2	D	56	ASP
2	D	60	LEU
2	D	65	LEU
2	D	82	LEU
2	D	89	ASN
2	D	100	LEU
2	D	101	THR
2	D	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1638	ASN
2	D	55	GLN

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)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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	PGE	A	1901	-	9,9,9	0.81	0	8,8,8	1.26	0
3	PGE	B	1901	-	9,9,9	0.48	0	8,8,8	1.32	0
6	AYE	A	1905	1,2	3,3,3	0.33	0	1,2,2	0.95	0
5	GOL	B	1904	-	5,5,5	0.37	0	5,5,5	0.21	0
8	EDO	B	1908	-	3,3,3	0.93	0	2,2,2	0.94	0
5	GOL	A	1904	-	5,5,5	0.31	0	5,5,5	0.28	0
3	PGE	C	201	-	9,9,9	0.55	0	8,8,8	1.29	0
3	PGE	B	1902	-	9,9,9	0.65	0	8,8,8	1.32	0
6	AYE	B	1910	1,2	3,3,3	0.34	0	1,2,2	0.90	0
7	CIT	B	1907	-	12,12,12	1.91	3 (25%)	17,17,17	1.55	2 (11%)
5	GOL	B	1906	-	5,5,5	0.38	0	5,5,5	0.44	0
5	GOL	A	1903	-	5,5,5	0.34	0	5,5,5	0.19	0
5	GOL	B	1905	-	5,5,5	0.35	0	5,5,5	0.39	0
8	EDO	B	1909	-	3,3,3	0.71	0	2,2,2	0.92	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	PGE	A	1901	-	-	5/7/7/7	-
3	PGE	B	1901	-	-	5/7/7/7	-
6	AYE	A	1905	1,2	-	0/1/1/1	-
5	GOL	B	1904	-	-	4/4/4/4	-
8	EDO	B	1908	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1904	-	-	2/4/4/4	-
3	PGE	C	201	-	-	4/7/7/7	-
3	PGE	B	1902	-	-	2/7/7/7	-
6	AYE	B	1910	1,2	-	0/1/1/1	-
7	CIT	B	1907	-	-	2/16/16/16	-
5	GOL	B	1906	-	-	2/4/4/4	-
5	GOL	A	1903	-	-	2/4/4/4	-
5	GOL	B	1905	-	-	3/4/4/4	-
8	EDO	B	1909	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1907	CIT	C3-C6	3.64	1.57	1.53
7	B	1907	CIT	C2-C3	2.87	1.57	1.53
7	B	1907	CIT	C4-C3	2.14	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1907	CIT	O5-C6-C3	-4.21	116.29	122.25
7	B	1907	CIT	O6-C6-C3	3.41	118.98	113.05

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1904	GOL	C1-C2-C3-O3
5	B	1904	GOL	O1-C1-C2-C3
5	B	1904	GOL	O2-C2-C3-O3
5	B	1905	GOL	O2-C2-C3-O3
3	C	201	PGE	O2-C3-C4-O3
3	B	1902	PGE	O2-C3-C4-O3
3	B	1901	PGE	O1-C1-C2-O2
5	B	1904	GOL	C1-C2-C3-O3
5	B	1905	GOL	C1-C2-C3-O3
5	B	1906	GOL	O1-C1-C2-C3
3	B	1901	PGE	O3-C5-C6-O4
3	C	201	PGE	O3-C5-C6-O4
5	A	1904	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	1904	GOL	O1-C1-C2-O2
5	B	1906	GOL	O1-C1-C2-O2
7	B	1907	CIT	C2-C3-C4-C5
7	B	1907	CIT	O7-C3-C4-C5
3	A	1901	PGE	O1-C1-C2-O2
3	A	1901	PGE	O3-C5-C6-O4
3	B	1902	PGE	O3-C5-C6-O4
3	C	201	PGE	O1-C1-C2-O2
3	B	1901	PGE	O2-C3-C4-O3
3	B	1901	PGE	C3-C4-O3-C5
5	A	1903	GOL	O1-C1-C2-O2
3	A	1901	PGE	C6-C5-O3-C4
5	B	1905	GOL	O1-C1-C2-C3
5	A	1903	GOL	O1-C1-C2-C3
3	C	201	PGE	C6-C5-O3-C4
3	A	1901	PGE	C3-C4-O3-C5
3	A	1901	PGE	O2-C3-C4-O3
3	B	1901	PGE	C6-C5-O3-C4

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1905	AYE	1	0
5	A	1904	GOL	1	0
3	B	1902	PGE	1	0
5	B	1906	GOL	4	0
5	B	1905	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	259/259 (100%)	-0.38	0 100 100	17, 29, 49, 57	0
1	B	259/259 (100%)	-0.43	0 100 100	18, 29, 49, 55	0
2	C	153/156 (98%)	0.88	30 (19%) 1 1	25, 61, 126, 133	0
2	D	153/156 (98%)	0.77	26 (16%) 1 2	23, 62, 121, 136	0
All	All	824/830 (99%)	0.05	56 (6%) 17 22	17, 36, 115, 136	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	66	GLY	14.3
2	D	22	SER	10.4
2	D	68	GLY	7.7
2	C	17	VAL	6.7
2	C	11	ALA	6.7
2	C	5	LEU	6.6
2	C	67	PRO	5.8
2	C	12	GLY	5.2
2	C	4	ASP	5.1
2	C	34	GLN	5.0
2	C	22	SER	4.9
2	D	20	SER	4.9
2	D	10	LEU	4.7
2	D	61	ALA	4.7
2	D	67	PRO	4.6
2	D	15	PHE	4.5
2	D	66	GLY	4.4
2	C	54	LEU	4.4
2	D	18	SER	4.4
2	D	19	LEU	4.4
2	C	18	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	65	LEU	3.8
2	D	60	LEU	3.7
2	D	34	GLN	3.6
2	D	9	MET	3.6
2	C	58	VAL	3.5
2	D	5	LEU	3.4
2	C	20	SER	3.3
2	C	68	GLY	3.2
2	C	19	LEU	2.9
2	C	16	GLN	2.9
2	D	11	ALA	2.9
2	D	65	LEU	2.9
2	D	63	GLN	2.8
2	C	15	PHE	2.8
2	C	60	LEU	2.8
2	C	57	ARG	2.6
2	C	21	SER	2.6
2	D	4	ASP	2.6
2	D	21	SER	2.5
2	C	13	ASN	2.4
2	C	28	LEU	2.4
2	D	33	THR	2.4
2	C	36	ILE	2.4
2	D	27	GLU	2.4
2	C	6	THR	2.3
2	D	52	VAL	2.3
2	D	17	VAL	2.3
2	D	62	SER	2.2
2	C	77	LYS	2.2
2	C	23	MET	2.2
2	C	38	VAL	2.1
2	D	6	THR	2.1
2	D	53	ALA	2.1
2	C	61	ALA	2.1
2	C	47	VAL	2.1

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^{th} 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
8	EDO	B	1909	4/4	0.80	0.26	50,62,75,81	0
7	CIT	B	1907	13/13	0.82	0.20	61,75,91,91	0
5	GOL	B	1905	6/6	0.82	0.23	33,49,59,59	0
5	GOL	B	1904	6/6	0.83	0.19	44,56,66,67	0
5	GOL	A	1904	6/6	0.83	0.26	32,46,64,64	0
3	PGE	A	1901	10/10	0.84	0.17	35,54,66,76	0
3	PGE	B	1902	10/10	0.86	0.19	51,65,78,84	0
5	GOL	B	1906	6/6	0.86	0.23	42,60,67,72	0
3	PGE	B	1901	10/10	0.87	0.15	42,55,67,69	0
5	GOL	A	1903	6/6	0.89	0.22	51,61,72,78	0
3	PGE	C	201	10/10	0.93	0.12	39,51,63,70	0
8	EDO	B	1908	4/4	0.95	0.11	31,40,56,67	0
6	AYE	B	1910	4/4	0.96	0.12	28,34,35,35	0
6	AYE	A	1905	4/4	0.96	0.10	29,35,37,37	0
4	ZN	A	1902	1/1	0.97	0.08	52,52,52,52	0
4	ZN	B	1903	1/1	0.98	0.09	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.