Full wwPDB X-ray Structure Validation Report (i)

Jul 21, 2022 – 04:11 pm BST

PDB ID	:	7PI6
Title	:	Trypanosoma brucei ISG65 bound to human complement C3d
Authors	:	Cook, A.D.; Higgins, M.K.
Deposited on	:	2021-08-19
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

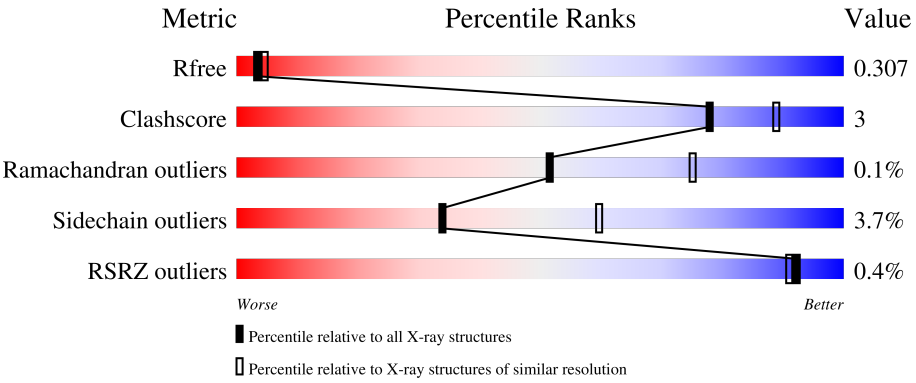
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	400	50% 6% 45%
1	C	400	% 44% 5% 51%
2	B	293	90% 9% .
2	D	293	88% 10% ..

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7957 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 65 kDa invariant surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1745	1088	304	347	6			
1	C	196	Total	C	N	O	S	0	0	0
			1546	965	269	308	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP Q587F5
A	23	ALA	-	expression tag	UNP Q587F5
A	33	ASN	LYS	conflict	UNP Q587F5
A	55	LYS	GLU	conflict	UNP Q587F5
A	111	ASP	ASN	conflict	UNP Q587F5
A	130	ASP	GLU	conflict	UNP Q587F5
A	140	GLU	LYS	conflict	UNP Q587F5
A	152	ASP	GLU	conflict	UNP Q587F5
A	153	HIS	TYR	conflict	UNP Q587F5
A	154	LYS	ARG	conflict	UNP Q587F5
A	174	SER	ARG	conflict	UNP Q587F5
A	188	ASN	LYS	conflict	UNP Q587F5
A	238	GLU	MET	conflict	UNP Q587F5
A	260	HIS	PRO	conflict	UNP Q587F5
A	266	LYS	GLU	conflict	UNP Q587F5
A	269	LYS	ARG	conflict	UNP Q587F5
A	273	GLY	ASP	conflict	UNP Q587F5
A	275	HIS	TYR	conflict	UNP Q587F5
A	276	GLU	GLN	conflict	UNP Q587F5
A	277	LYS	ARG	conflict	UNP Q587F5
A	279	ARG	LYS	conflict	UNP Q587F5
A	280	ARG	LYS	conflict	UNP Q587F5
A	306	ALA	THR	conflict	UNP Q587F5
A	314	GLU	ASP	conflict	UNP Q587F5
A	330	VAL	ALA	conflict	UNP Q587F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	343	PRO	SER	conflict	UNP Q587F5
A	368	GLY	SER	conflict	UNP Q587F5
A	371	GLU	ASP	conflict	UNP Q587F5
A	373	ALA	THR	conflict	UNP Q587F5
A	384	LYS	ARG	conflict	UNP Q587F5
A	386	GLY	-	expression tag	UNP Q587F5
A	387	SER	-	expression tag	UNP Q587F5
A	388	GLY	-	expression tag	UNP Q587F5
A	389	SER	-	expression tag	UNP Q587F5
A	390	GLY	-	expression tag	UNP Q587F5
A	391	SER	-	expression tag	UNP Q587F5
A	392	ALA	-	expression tag	UNP Q587F5
A	393	SER	-	expression tag	UNP Q587F5
A	394	GLY	-	expression tag	UNP Q587F5
A	395	GLY	-	expression tag	UNP Q587F5
A	396	LEU	-	expression tag	UNP Q587F5
A	397	ASN	-	expression tag	UNP Q587F5
A	398	ASP	-	expression tag	UNP Q587F5
A	399	ILE	-	expression tag	UNP Q587F5
A	400	PHE	-	expression tag	UNP Q587F5
A	401	GLU	-	expression tag	UNP Q587F5
A	402	ALA	-	expression tag	UNP Q587F5
A	403	GLN	-	expression tag	UNP Q587F5
A	404	LYS	-	expression tag	UNP Q587F5
A	405	ILE	-	expression tag	UNP Q587F5
A	406	GLU	-	expression tag	UNP Q587F5
A	407	TRP	-	expression tag	UNP Q587F5
A	408	HIS	-	expression tag	UNP Q587F5
A	409	GLU	-	expression tag	UNP Q587F5
A	410	GLY	-	expression tag	UNP Q587F5
A	411	GLY	-	expression tag	UNP Q587F5
A	412	HIS	-	expression tag	UNP Q587F5
A	413	HIS	-	expression tag	UNP Q587F5
A	414	HIS	-	expression tag	UNP Q587F5
A	415	HIS	-	expression tag	UNP Q587F5
A	416	HIS	-	expression tag	UNP Q587F5
A	417	HIS	-	expression tag	UNP Q587F5
A	418	HIS	-	expression tag	UNP Q587F5
A	419	HIS	-	expression tag	UNP Q587F5
A	420	HIS	-	expression tag	UNP Q587F5
A	421	HIS	-	expression tag	UNP Q587F5
C	22	ALA	-	expression tag	UNP Q587F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	ALA	-	expression tag	UNP Q587F5
C	33	ASN	LYS	conflict	UNP Q587F5
C	55	LYS	GLU	conflict	UNP Q587F5
C	111	ASP	ASN	conflict	UNP Q587F5
C	130	ASP	GLU	conflict	UNP Q587F5
C	140	GLU	LYS	conflict	UNP Q587F5
C	152	ASP	GLU	conflict	UNP Q587F5
C	153	HIS	TYR	conflict	UNP Q587F5
C	154	LYS	ARG	conflict	UNP Q587F5
C	174	SER	ARG	conflict	UNP Q587F5
C	188	ASN	LYS	conflict	UNP Q587F5
C	238	GLU	MET	conflict	UNP Q587F5
C	260	HIS	PRO	conflict	UNP Q587F5
C	266	LYS	GLU	conflict	UNP Q587F5
C	269	LYS	ARG	conflict	UNP Q587F5
C	273	GLY	ASP	conflict	UNP Q587F5
C	275	HIS	TYR	conflict	UNP Q587F5
C	276	GLU	GLN	conflict	UNP Q587F5
C	277	LYS	ARG	conflict	UNP Q587F5
C	279	ARG	LYS	conflict	UNP Q587F5
C	280	ARG	LYS	conflict	UNP Q587F5
C	306	ALA	THR	conflict	UNP Q587F5
C	314	GLU	ASP	conflict	UNP Q587F5
C	330	VAL	ALA	conflict	UNP Q587F5
C	343	PRO	SER	conflict	UNP Q587F5
C	368	GLY	SER	conflict	UNP Q587F5
C	371	GLU	ASP	conflict	UNP Q587F5
C	373	ALA	THR	conflict	UNP Q587F5
C	384	LYS	ARG	conflict	UNP Q587F5
C	386	GLY	-	expression tag	UNP Q587F5
C	387	SER	-	expression tag	UNP Q587F5
C	388	GLY	-	expression tag	UNP Q587F5
C	389	SER	-	expression tag	UNP Q587F5
C	390	GLY	-	expression tag	UNP Q587F5
C	391	SER	-	expression tag	UNP Q587F5
C	392	ALA	-	expression tag	UNP Q587F5
C	393	SER	-	expression tag	UNP Q587F5
C	394	GLY	-	expression tag	UNP Q587F5
C	395	GLY	-	expression tag	UNP Q587F5
C	396	LEU	-	expression tag	UNP Q587F5
C	397	ASN	-	expression tag	UNP Q587F5
C	398	ASP	-	expression tag	UNP Q587F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	399	ILE	-	expression tag	UNP Q587F5
C	400	PHE	-	expression tag	UNP Q587F5
C	401	GLU	-	expression tag	UNP Q587F5
C	402	ALA	-	expression tag	UNP Q587F5
C	403	GLN	-	expression tag	UNP Q587F5
C	404	LYS	-	expression tag	UNP Q587F5
C	405	ILE	-	expression tag	UNP Q587F5
C	406	GLU	-	expression tag	UNP Q587F5
C	407	TRP	-	expression tag	UNP Q587F5
C	408	HIS	-	expression tag	UNP Q587F5
C	409	GLU	-	expression tag	UNP Q587F5
C	410	GLY	-	expression tag	UNP Q587F5
C	411	GLY	-	expression tag	UNP Q587F5
C	412	HIS	-	expression tag	UNP Q587F5
C	413	HIS	-	expression tag	UNP Q587F5
C	414	HIS	-	expression tag	UNP Q587F5
C	415	HIS	-	expression tag	UNP Q587F5
C	416	HIS	-	expression tag	UNP Q587F5
C	417	HIS	-	expression tag	UNP Q587F5
C	418	HIS	-	expression tag	UNP Q587F5
C	419	HIS	-	expression tag	UNP Q587F5
C	420	HIS	-	expression tag	UNP Q587F5
C	421	HIS	-	expression tag	UNP Q587F5

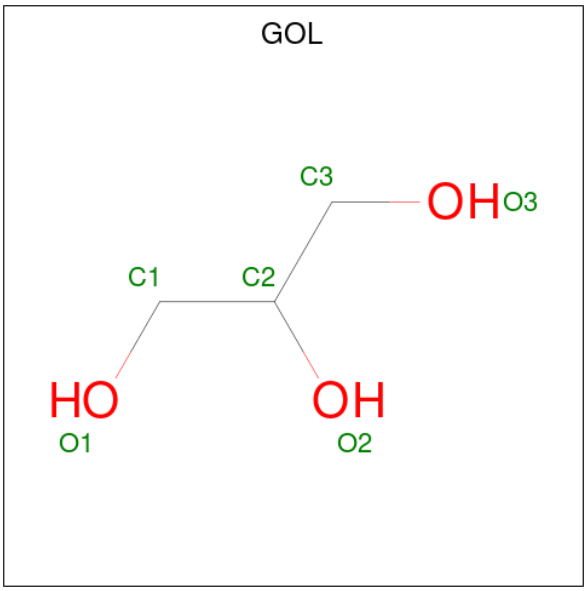
- Molecule 2 is a protein called Complement C3dg fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	290	Total	C	N	O	S	0	0	0
			2288	1471	384	424	9			
2	D	289	Total	C	N	O	S	0	0	0
			2280	1467	383	421	9			

There are 4 discrepancies between the modelled and reference sequences:

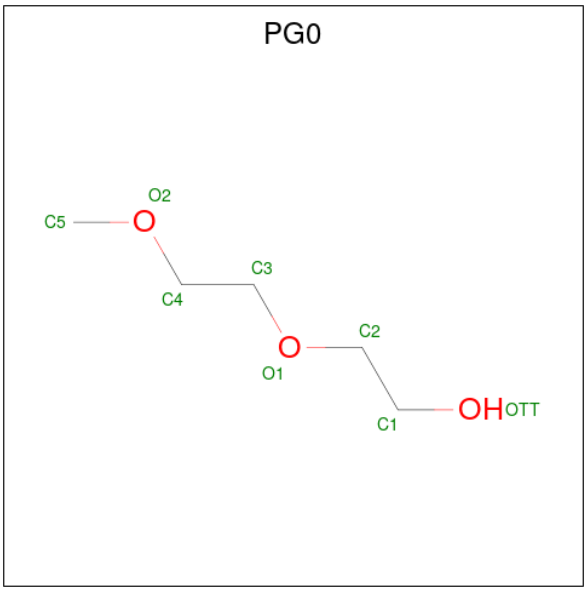
Chain	Residue	Modelled	Actual	Comment	Reference
B	995	GLY	-	expression tag	UNP P01024
B	1010	ALA	CYS	conflict	UNP P01024
D	995	GLY	-	expression tag	UNP P01024
D	1010	ALA	CYS	conflict	UNP P01024

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 8 5 3	0	0

- Molecule 5 is water.

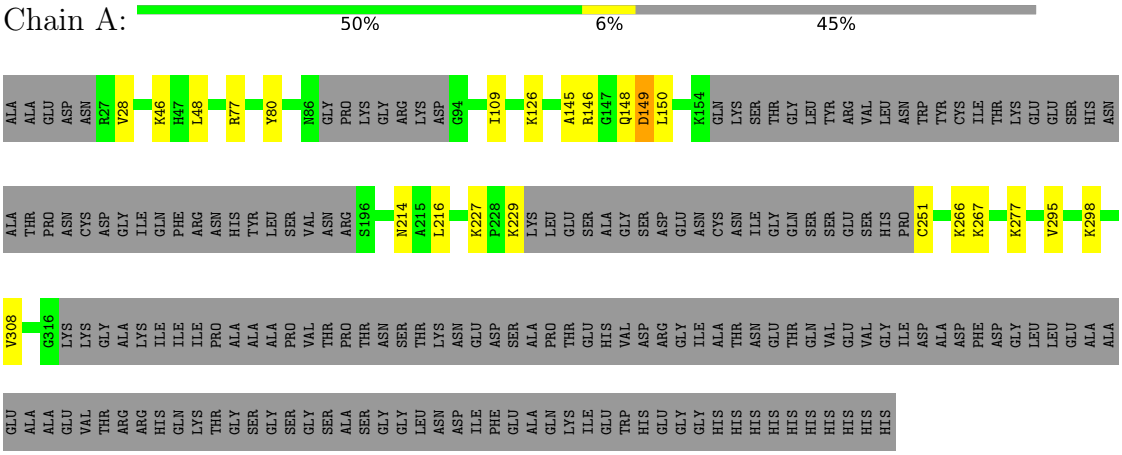
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	18	Total O 18 18	0	0
5	C	6	Total O 6 6	0	0
5	D	19	Total O 19 19	0	0

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.

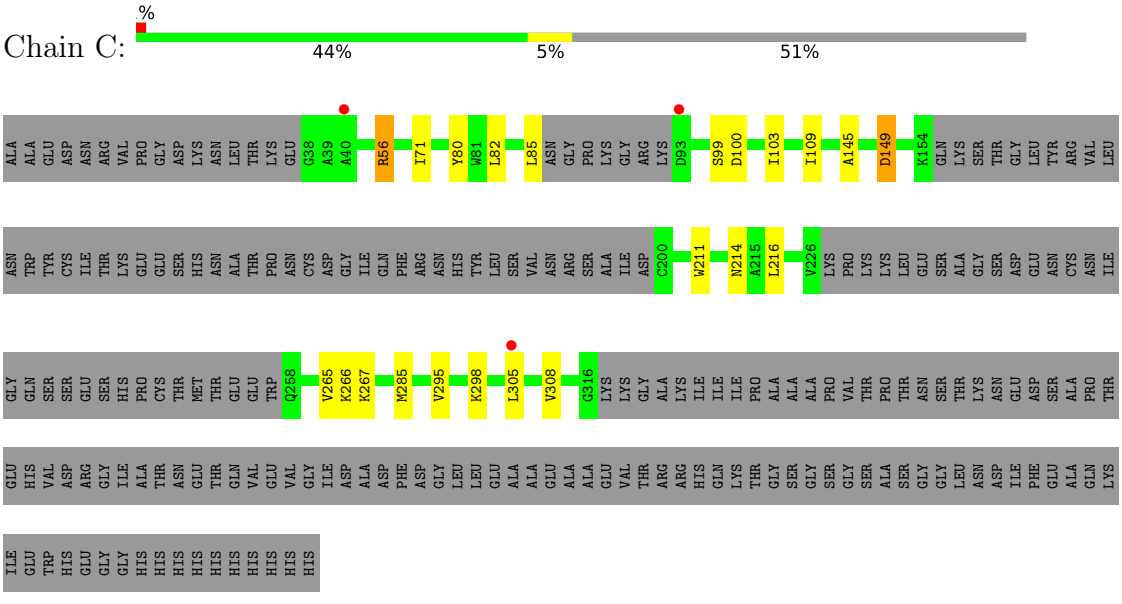
• Molecule 1: 65 kDa invariant surface glycoprotein

Chain A:



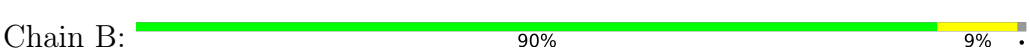
• Molecule 1: 65 kDa invariant surface glycoprotein

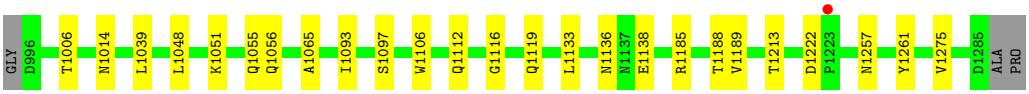
Chain C:



• Molecule 2: Complement C3dg fragment

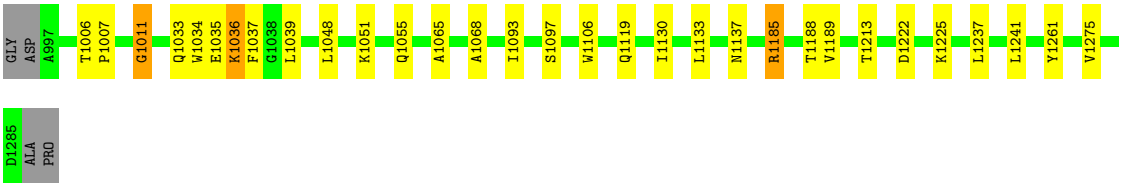
Chain B:





• Molecule 2: Complement C3dg fragment

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.95Å 189.58Å 73.88Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	94.79 – 2.60 94.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (94.79-2.60) 98.0 (94.79-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-APR-2021)	Depositor
R, R_{free}	0.268 , 0.310 0.262 , 0.307	Depositor DCC
R_{free} test set	2065 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.286 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7957	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: PG0, GOL

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	0.34	0/1771	0.49	0/2375
1	C	0.33	0/1568	0.48	0/2101
2	B	0.39	0/2336	0.58	0/3164
2	D	0.38	0/2328	0.59	1/3153 (0.0%)
All	All	0.37	0/8003	0.54	1/10793 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1185	ARG	CD-NE-CZ	5.52	131.32	123.60

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	1745	0	1709	9	0
1	C	1546	0	1507	10	0
2	B	2288	0	2294	10	0
2	D	2280	0	2290	16	0
3	A	6	0	8	0	0
3	B	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	0	0
3	D	6	0	8	1	0
4	D	8	0	12	0	0
5	A	17	0	0	0	0
5	B	18	0	0	0	0
5	C	6	0	0	0	0
5	D	19	0	0	0	0
All	All	7957	0	7852	45	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 3.

All (45) 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:1137:ASN:O	2:D:1185:ARG:NH1	2.06	0.88
2:D:1033:GLN:HA	2:D:1036:LYS:HE2	1.67	0.77
1:C:56:ARG:HG3	1:C:211:TRP:HB2	1.74	0.69
2:B:1257:ASN:HA	3:B:1300:GOL:H31	1.76	0.67
2:B:1257:ASN:HA	3:B:1300:GOL:C3	2.27	0.65
1:C:145:ALA:O	1:C:149:ASP:HB2	1.96	0.64
2:D:1051:LYS:NZ	2:D:1055:GLN:NE2	2.50	0.59
2:D:1007:PRO:HD2	2:D:1051:LYS:HD3	1.85	0.58
2:B:1112:GLN:HE21	2:B:1116:GLY:HA2	1.69	0.57
1:C:71:ILE:HG12	1:C:285:MET:HE2	1.87	0.56
2:D:1051:LYS:HZ3	2:D:1055:GLN:NE2	2.05	0.54
2:D:1034:TRP:O	2:D:1037:PHE:O	2.24	0.54
1:A:109:ILE:HG21	1:A:295:VAL:HG21	1.91	0.53
2:B:1261:TYR:HD2	2:B:1275:VAL:HG11	1.74	0.52
1:A:145:ALA:O	1:A:149:ASP:HB2	2.10	0.51
2:D:1051:LYS:O	2:D:1055:GLN:HG3	2.10	0.51
1:C:109:ILE:HG21	1:C:295:VAL:HG21	1.91	0.51
2:B:1051:LYS:O	2:B:1055:GLN:HG3	2.13	0.49
1:A:266:LYS:NZ	1:A:267:LYS:HE3	2.28	0.48
1:C:266:LYS:NZ	1:C:267:LYS:HE3	2.29	0.48
2:B:1065:ALA:HB2	2:B:1106:TRP:CD2	2.48	0.48
1:A:48:LEU:HD13	1:A:216:LEU:HA	1.97	0.47
2:D:1011:GLY:HA3	2:D:1068:ALA:HA	1.96	0.47
1:C:216:LEU:HB3	1:C:265:VAL:HG22	1.97	0.47
1:A:227:LYS:NZ	1:A:229:LYS:HD3	2.30	0.47
1:A:46:LYS:HD2	1:A:150:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1065:ALA:HB2	2:D:1106:TRP:CD2	2.49	0.46
2:D:1051:LYS:HZ2	2:D:1055:GLN:HE22	1.63	0.46
2:D:1189:VAL:HG11	2:D:1213:THR:OG1	2.16	0.44
2:B:1138:GLU:H	2:B:1185:ARG:HH11	1.65	0.43
2:B:1189:VAL:HG11	2:B:1213:THR:OG1	2.18	0.43
2:D:1261:TYR:HD2	2:D:1275:VAL:HG11	1.83	0.43
2:D:1237:LEU:O	2:D:1241:LEU:HG	2.19	0.42
1:C:99:SER:O	1:C:103:ILE:HG13	2.20	0.42
2:D:1051:LYS:HZ3	2:D:1055:GLN:CD	2.23	0.42
1:A:146:ARG:HG2	1:A:146:ARG:O	2.19	0.42
2:B:1014:ASN:HB3	2:B:1056:GLN:OE1	2.20	0.42
1:C:298:LYS:HB3	1:C:308:VAL:HG12	2.02	0.42
1:A:126:LYS:HD3	1:A:277:LYS:HE2	2.02	0.41
1:A:298:LYS:HB3	1:A:308:VAL:HG12	2.02	0.41
1:C:82:LEU:HA	1:C:85:LEU:HD12	2.03	0.41
2:B:1006:THR:HA	2:B:1048:LEU:HD22	2.03	0.41
1:C:100:ASP:HA	1:C:103:ILE:HD12	2.03	0.41
2:D:1006:THR:HA	2:D:1048:LEU:HD22	2.03	0.41
2:D:1130:ILE:HD13	3:D:1300:GOL:H12	2.04	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	213/400 (53%)	207 (97%)	6 (3%)	0	100	100
1	C	188/400 (47%)	183 (97%)	5 (3%)	0	100	100
2	B	288/293 (98%)	277 (96%)	11 (4%)	0	100	100
2	D	287/293 (98%)	274 (96%)	12 (4%)	1 (0%)	41	64
All	All	976/1386 (70%)	941 (96%)	34 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1011	GLY

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	178/323 (55%)	171 (96%)	7 (4%)	32	58
1	C	155/323 (48%)	150 (97%)	5 (3%)	39	65
2	B	240/241 (100%)	232 (97%)	8 (3%)	38	64
2	D	239/241 (99%)	229 (96%)	10 (4%)	30	55
All	All	812/1128 (72%)	782 (96%)	30 (4%)	34	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	77	ARG
1	A	80	TYR
1	A	148	GLN
1	A	149	ASP
1	A	214	ASN
1	A	251	CYS
2	B	1039	LEU
2	B	1093	ILE
2	B	1097	SER
2	B	1119	GLN
2	B	1133	LEU
2	B	1136	ASN
2	B	1188	THR
2	B	1222	ASP
1	C	56	ARG
1	C	80	TYR
1	C	149	ASP
1	C	214	ASN

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Mol	Chain	Res	Type
1	C	305	LEU
2	D	1035	GLU
2	D	1036	LYS
2	D	1039	LEU
2	D	1093	ILE
2	D	1097	SER
2	D	1119	GLN
2	D	1133	LEU
2	D	1188	THR
2	D	1222	ASP
2	D	1225	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1055	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)

6 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	GOL	D	1300	-	5,5,5	0.08	0	5,5,5	0.20	0
3	GOL	C	501	-	5,5,5	0.03	0	5,5,5	0.17	0
3	GOL	B	1301	-	5,5,5	0.11	0	5,5,5	0.26	0
3	GOL	B	1300	-	5,5,5	0.05	0	5,5,5	0.07	0
4	PG0	D	1301	-	7,7,7	0.26	0	6,6,6	0.26	0
3	GOL	A	501	-	5,5,5	0.05	0	5,5,5	0.20	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	GOL	D	1300	-	-	1/4/4/4	-
3	GOL	C	501	-	-	0/4/4/4	-
3	GOL	B	1301	-	-	1/4/4/4	-
3	GOL	B	1300	-	-	0/4/4/4	-
4	PG0	D	1301	-	-	2/5/5/5	-
3	GOL	A	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GOL	C1-C2-C3-O3
3	D	1300	GOL	O1-C1-C2-C3
3	A	501	GOL	O2-C2-C3-O3
4	D	1301	PG0	OTT-C1-C2-O1
4	D	1301	PG0	C4-C3-O1-C2
3	B	1301	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1300	GOL	1	0
3	B	1300	GOL	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^{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	221/400 (55%)	-0.00	0 100 100	33, 56, 73, 79	0
1	C	196/400 (49%)	0.21	3 (1%) 73 70	31, 65, 85, 96	0
2	B	290/293 (98%)	-0.11	1 (0%) 94 93	29, 43, 62, 72	0
2	D	289/293 (98%)	-0.14	0 100 100	28, 43, 60, 75	0
All	All	996/1386 (71%)	-0.03	4 (0%) 92 91	28, 48, 76, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1223	PRO	2.7
1	C	305	LEU	2.3
1	C	40	ALA	2.3
1	C	93	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	GOL	B	1301	6/6	0.82	0.21	46,47,48,48	0
3	GOL	A	501	6/6	0.91	0.32	63,64,64,64	0
3	GOL	C	501	6/6	0.91	0.27	85,85,85,85	0
3	GOL	D	1300	6/6	0.94	0.25	40,41,42,42	0
3	GOL	B	1300	6/6	0.95	0.16	68,68,69,69	0
4	PG0	D	1301	8/8	0.96	0.26	45,46,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.