Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:51 AM EDT

PDB ID	:	6GEL
Title	:	The structure of TWITCH-2B
Authors	:	Trigo Mourino, P.; Paulat, M.; Thestrup, T.; Griesbeck, O.; Griesinger, C.; Becker, S.
Deposited on	:	2018-04-26
Resolution	:	2.51 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:

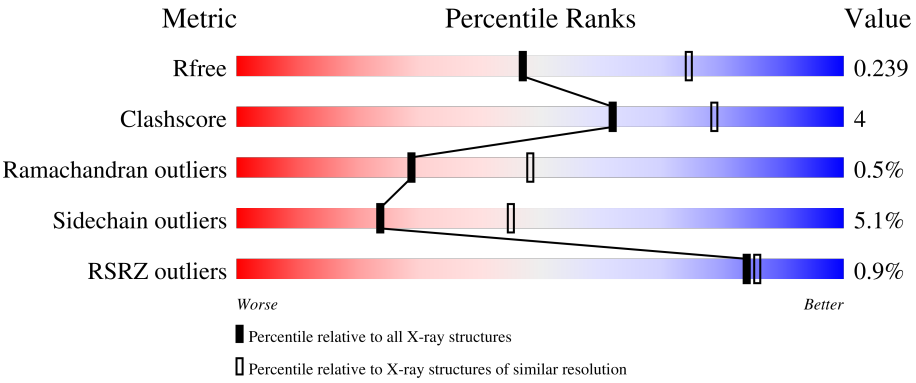
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.51 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 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	552	% 86% 9%
1	B	552	% 82% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8685 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 Green fluorescent protein,Optimized Ratiometric Calcium Sensor,Green fluorescent protein,Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	3	0
			4278	2710	720	832	16			
1	B	530	Total	C	N	O	S	0	1	0
			4249	2696	713	823	17			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP P42212
A	65	LEU	PHE	conflict	UNP P42212
A	66	CRF	SER	chromophore	UNP P42212
A	66	CRF	TYR	chromophore	UNP P42212
A	66	CRF	GLY	chromophore	UNP P42212
A	73	ALA	SER	conflict	UNP P42212
A	146	ALA	TYR	conflict	UNP P42212
A	147	ILE	ASN	conflict	UNP P42212
A	148	HIS	SER	conflict	UNP P42212
A	149	GLY	HIS	conflict	UNP P42212
A	154	THR	MET	conflict	UNP P42212
A	164	ALA	VAL	conflict	UNP P42212
A	167	GLY	LYS	conflict	UNP P42212
A	168	LEU	ILE	conflict	UNP P42212
A	169	ASN	ARG	conflict	UNP P42212
A	170	CYS	HIS	conflict	UNP P42212
A	207	LYS	ALA	conflict	UNP P42212
A	229	ARG	-	linker	UNP P42212
A	230	MET	-	linker	UNP P42212
A	231	GLN	-	linker	UNP P42212
A	232	VAL	-	linker	UNP P42212
A	233	ALA	-	linker	UNP P42212
A	234	ASP	-	linker	UNP P42212
A	235	ALA	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	249	PHE	LYS	conflict	UNP W5IDB2
A	300	VAL	MET	conflict	UNP W5IDB2
A	305	PRO	-	linker	UNP W5IDB2
A	306	ILE	-	linker	UNP W5IDB2
A	307	TYR	-	linker	UNP W5IDB2
A	308	PRO	-	linker	UNP W5IDB2
A	309	GLU	-	linker	UNP W5IDB2
A	310	LEU	-	linker	UNP W5IDB2
A	311	MET	-	linker	UNP W5IDB2
A	313	GLY	SER	conflict	UNP P42212
A	341	TYR	THR	conflict	UNP P42212
A	344	LYS	ALA	conflict	UNP P42212
A	369	LEU	HIS	conflict	UNP P42212
A	377	GLY	-	linker	UNP P42212
A	378	GLY	-	linker	UNP P42212
A	379	THR	-	linker	UNP P42212
A	380	GLY	-	linker	UNP P42212
A	381	GLY	-	linker	UNP P42212
A	382	SER	-	linker	UNP P42212
A	384	VAL	-	insertion	UNP P42212
A	413	ARG	SER	conflict	UNP P42212
A	422	ASN	TYR	conflict	UNP P42212
A	429	LEU	PHE	conflict	UNP P42212
A	447	LEU	PHE	conflict	UNP P42212
A	448	CR2	SER	chromophore	UNP P42212
A	448	CR2	TYR	chromophore	UNP P42212
A	448	CR2	GLY	chromophore	UNP P42212
A	451	LEU	VAL	conflict	UNP P42212
A	452	MET	GLN	conflict	UNP P42212
A	455	ALA	SER	conflict	UNP P42212
A	536	THR	MET	conflict	UNP P42212
A	546	ALA	VAL	conflict	UNP P42212
B	2	VAL	-	insertion	UNP P42212
B	65	LEU	PHE	conflict	UNP P42212
B	66	CRF	SER	chromophore	UNP P42212
B	66	CRF	TYR	chromophore	UNP P42212
B	66	CRF	GLY	chromophore	UNP P42212
B	73	ALA	SER	conflict	UNP P42212
B	146	ALA	TYR	conflict	UNP P42212
B	147	ILE	ASN	conflict	UNP P42212
B	148	HIS	SER	conflict	UNP P42212
B	149	GLY	HIS	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	154	THR	MET	conflict	UNP P42212
B	164	ALA	VAL	conflict	UNP P42212
B	167	GLY	LYS	conflict	UNP P42212
B	168	LEU	ILE	conflict	UNP P42212
B	169	ASN	ARG	conflict	UNP P42212
B	170	CYS	HIS	conflict	UNP P42212
B	207	LYS	ALA	conflict	UNP P42212
B	229	ARG	-	linker	UNP P42212
B	230	MET	-	linker	UNP P42212
B	231	GLN	-	linker	UNP P42212
B	232	VAL	-	linker	UNP P42212
B	233	ALA	-	linker	UNP P42212
B	234	ASP	-	linker	UNP P42212
B	235	ALA	-	linker	UNP P42212
B	249	PHE	LYS	conflict	UNP W5IDB2
B	300	VAL	MET	conflict	UNP W5IDB2
B	305	PRO	-	linker	UNP W5IDB2
B	306	ILE	-	linker	UNP W5IDB2
B	307	TYR	-	linker	UNP W5IDB2
B	308	PRO	-	linker	UNP W5IDB2
B	309	GLU	-	linker	UNP W5IDB2
B	310	LEU	-	linker	UNP W5IDB2
B	311	MET	-	linker	UNP W5IDB2
B	313	GLY	SER	conflict	UNP P42212
B	341	TYR	THR	conflict	UNP P42212
B	344	LYS	ALA	conflict	UNP P42212
B	369	LEU	HIS	conflict	UNP P42212
B	377	GLY	-	linker	UNP P42212
B	378	GLY	-	linker	UNP P42212
B	379	THR	-	linker	UNP P42212
B	380	GLY	-	linker	UNP P42212
B	381	GLY	-	linker	UNP P42212
B	382	SER	-	linker	UNP P42212
B	384	VAL	-	insertion	UNP P42212
B	413	ARG	SER	conflict	UNP P42212
B	422	ASN	TYR	conflict	UNP P42212
B	429	LEU	PHE	conflict	UNP P42212
B	447	LEU	PHE	conflict	UNP P42212
B	448	CR2	SER	chromophore	UNP P42212
B	448	CR2	TYR	chromophore	UNP P42212
B	448	CR2	GLY	chromophore	UNP P42212
B	451	LEU	VAL	conflict	UNP P42212

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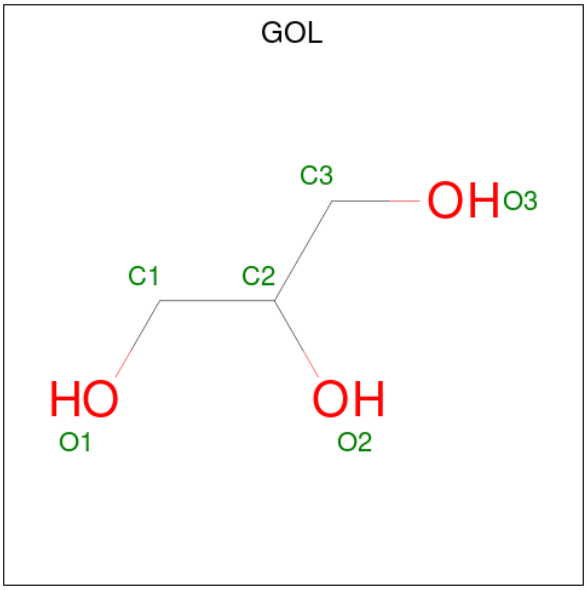
Chain	Residue	Modelled	Actual	Comment	Reference
B	452	MET	GLN	conflict	UNP P42212
B	455	ALA	SER	conflict	UNP P42212
B	536	THR	MET	conflict	UNP P42212
B	546	ALA	VAL	conflict	UNP P42212

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

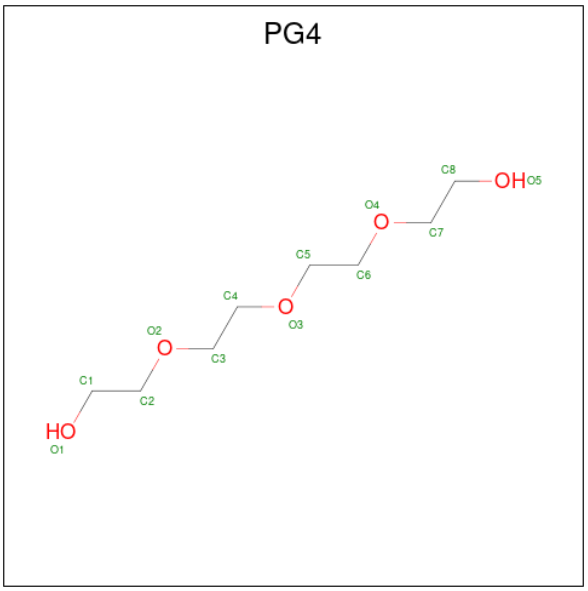
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0

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



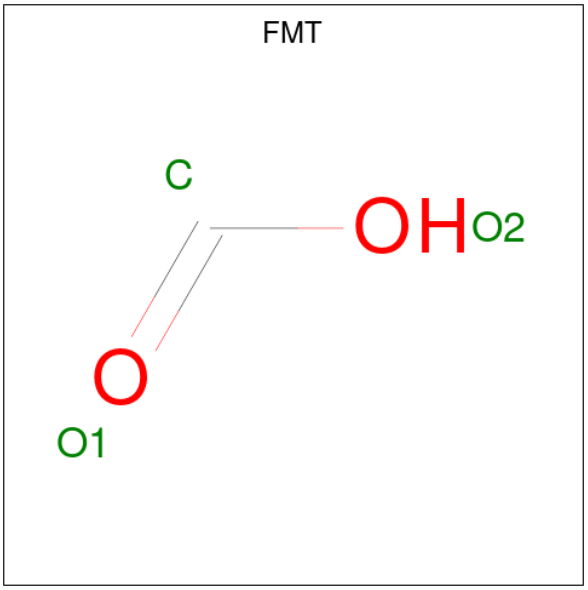
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	A	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0

- Molecule 6 is water.

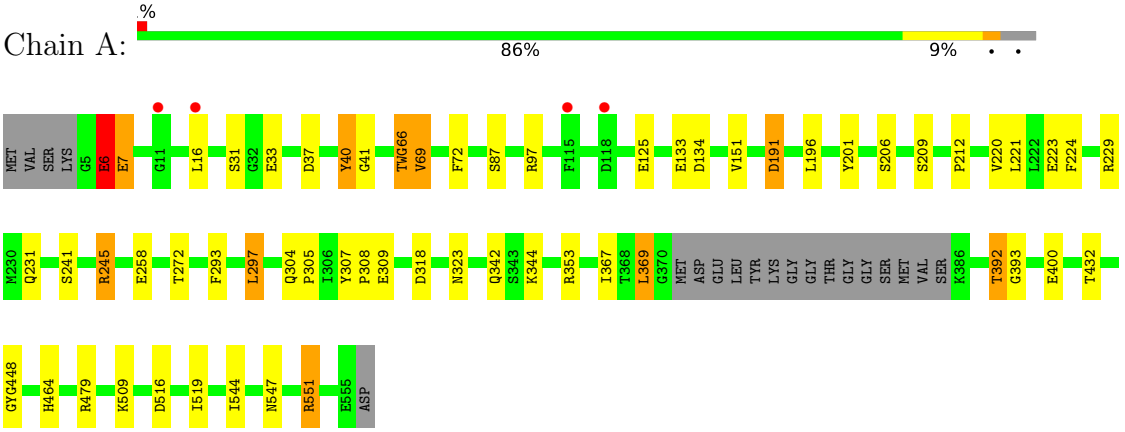
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	B	47	Total O 47 47	0	0

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.

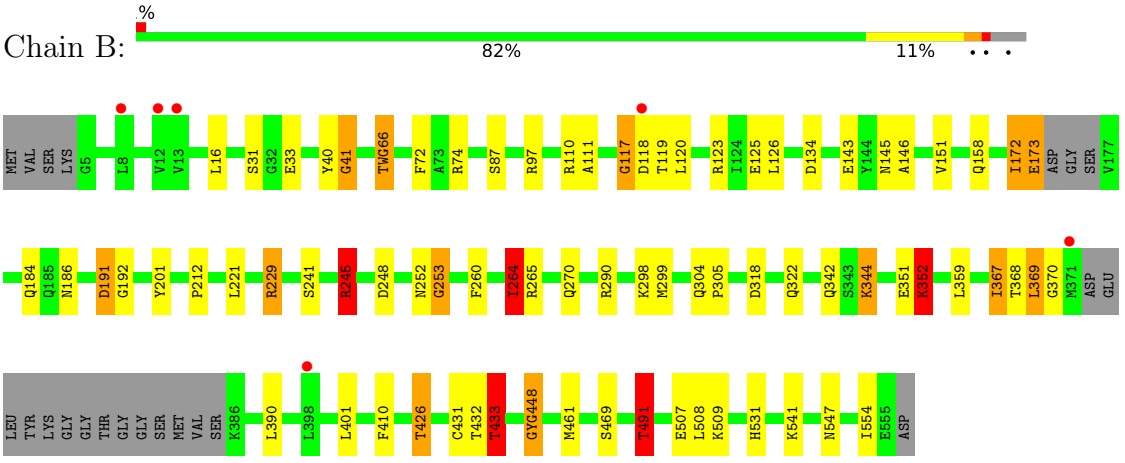
• Molecule 1: Green fluorescent protein,Optimized Ratiometric Calcium Sensor,Green fluorescent protein,Green fluorescent protein

Chain A:



• Molecule 1: Green fluorescent protein,Optimized Ratiometric Calcium Sensor,Green fluorescent protein,Green fluorescent protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.08Å 156.77Å 169.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.51 47.89 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.93-2.51) 98.7 (47.89-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.195 , 0.240 0.199 , 0.239	Depositor DCC
R_{free} test set	2656 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8685	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 2.85% 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: CRF, PG4, CA, FMT, CR2, 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	0.86	4/4323 (0.1%)	0.94	7/5837 (0.1%)
1	B	0.86	4/4293 (0.1%)	0.97	10/5795 (0.2%)
All	All	0.86	8/8616 (0.1%)	0.96	17/11632 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	10
All	All	0	15

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	GLY	N-CA	-8.50	1.33	1.46
1	B	173	GLU	N-CA	5.75	1.57	1.46
1	A	400	GLU	CD-OE1	5.63	1.31	1.25
1	A	133	GLU	CD-OE2	5.31	1.31	1.25
1	B	125	GLU	CD-OE1	5.29	1.31	1.25
1	B	125	GLU	CD-OE2	5.03	1.31	1.25
1	A	309	GLU	C-O	-5.02	1.13	1.23
1	A	125	GLU	CD-OE1	5.00	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97	ARG	NE-CZ-NH2	-7.57	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	479	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	145	ASN	CB-CA-C	-6.29	97.82	110.40
1	A	353	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	97	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	433	THR	CA-CB-OG1	-6.14	96.10	109.00
1	B	245[A]	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	245[B]	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	551	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	264	ILE	N-CA-CB	5.47	123.38	110.80
1	A	392	THR	C-N-CA	5.45	133.74	122.30
1	B	433	THR	OG1-CB-CG2	5.31	122.22	110.00
1	A	40	TYR	C-N-CA	-5.23	111.31	122.30
1	B	352	LYS	CB-CA-C	5.12	120.64	110.40
1	B	117	GLY	C-N-CA	5.09	134.44	121.70
1	B	491	THR	N-CA-CB	-5.09	100.62	110.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ARG	Sidechain
1	A	369	LEU	Peptide
1	A	392	THR	Peptide
1	A	393	GLY	Peptide
1	A	551	ARG	Sidechain
1	B	110	ARG	Sidechain
1	B	192	GLY	Peptide
1	B	229	ARG	Sidechain
1	B	245[A]	ARG	Sidechain
1	B	252	ASN	Peptide,Mainchain
1	B	290	ARG	Sidechain
1	B	40	TYR	Peptide,Mainchain
1	B	554	ILE	Peptide

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	4278	0	4117	29	0
1	B	4249	0	4098	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
4	A	8	0	10	1	0
5	A	6	0	2	0	0
5	B	9	0	3	0	0
6	A	66	0	0	1	0
6	B	47	0	0	5	0
All	All	8685	0	8254	74	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 4.

All (74) 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:B:241:SER:O	1:B:245[A]:ARG:HG3	1.78	0.82
1:B:410:PHE:HA	1:B:433:THR:HG21	1.66	0.76
1:A:209:SER:OG	1:A:220:VAL:CG1	2.35	0.74
1:B:184:GLN:HE21	1:B:186:ASN:HD21	1.37	0.72
1:B:352:LYS:H	1:B:352:LYS:CE	2.04	0.70
1:B:260:PHE:CE1	1:B:299:MET:HE1	2.27	0.69
1:A:241:SER:O	1:A:245:ARG:HG3	1.93	0.68
1:B:491:THR:HG21	6:B:718:HOH:O	1.95	0.66
1:B:260:PHE:CE1	1:B:299:MET:CE	2.78	0.66
1:A:66:CRF:HG11	1:A:221:LEU:HD21	1.77	0.65
1:B:509:LYS:HE2	6:B:701:HOH:O	1.96	0.65
1:A:241:SER:OG	1:A:245:ARG:NH1	2.31	0.64
1:B:41:GLY:H	1:B:74:ARG:HB2	1.62	0.63
1:A:209:SER:OG	1:A:220:VAL:HG13	1.99	0.63
1:B:66:CRF:HG11	1:B:221:LEU:HD21	1.81	0.63
1:B:352:LYS:H	1:B:352:LYS:HE2	1.63	0.63
1:B:491:THR:CG2	6:B:707:HOH:O	2.47	0.61
1:A:432:THR:O	1:B:245[A]:ARG:HD3	2.00	0.61
1:B:248:ASP:OD2	1:B:253:GLY:HA2	2.02	0.59
1:A:367:ILE:HD13	1:A:464:HIS:CD2	2.38	0.58
1:A:66:CRF:N2	1:A:66:CRF:HG12	2.19	0.57
1:B:448:CR2:HOH	1:B:531:HIS:HD1	1.52	0.57
1:B:66:CRF:HG11	1:B:221:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:THR:HG23	6:B:707:HOH:O	2.08	0.53
1:B:352:LYS:H	1:B:352:LYS:CD	2.21	0.52
1:B:410:PHE:CA	1:B:433:THR:HG21	2.37	0.52
1:A:206:SER:OG	1:A:223:GLU:OE1	2.25	0.52
1:B:191:ASP:N	1:B:191:ASP:OD1	2.43	0.51
1:B:143:GLU:HG3	1:B:172:ILE:O	2.11	0.50
1:B:241:SER:O	1:B:245[A]:ARG:CG	2.55	0.50
1:B:368:THR:HG23	1:B:370:GLY:H	1.77	0.49
1:B:431:CYS:SG	1:B:433:THR:HG22	2.52	0.49
1:B:241:SER:OG	1:B:245[A]:ARG:NH1	2.41	0.49
1:B:351:GLU:HA	1:B:352:LYS:HE2	1.95	0.49
1:A:509:LYS:HE2	6:A:701:HOH:O	2.12	0.48
1:A:69:VAL:HG13	1:A:72:PHE:HD2	1.78	0.48
1:B:72:PHE:CE2	1:B:120:LEU:HD22	2.48	0.48
1:B:367:ILE:HG12	1:B:461:MET:HG2	1.96	0.48
1:B:260:PHE:CE1	1:B:299:MET:HE2	2.48	0.48
1:A:66:CRF:N2	1:A:66:CRF:HD1	2.28	0.48
1:A:37:ASP:O	1:A:40:TYR:O	2.33	0.47
1:B:66:CRF:HD1	1:B:66:CRF:N2	2.29	0.46
1:B:245[B]:ARG:NH1	6:B:704:HOH:O	2.45	0.46
1:A:323:ASN:HB2	1:A:544:ILE:HG13	1.98	0.46
1:A:41:GLY:O	1:A:224:PHE:HA	2.16	0.46
1:B:359:LEU:HD13	1:B:426:THR:HG23	1.98	0.46
1:A:6:GLU:CD	1:A:6:GLU:N	2.70	0.45
1:A:7:GLU:HA	1:A:7:GLU:OE1	2.16	0.45
1:A:293:PHE:O	1:A:297:LEU:HD22	2.16	0.45
1:B:322:GLN:NE2	1:B:541:LYS:HD3	2.32	0.45
1:B:264:ILE:HD12	1:B:265:ARG:N	2.31	0.45
1:B:352:LYS:CD	1:B:352:LYS:N	2.80	0.44
1:A:191:ASP:N	1:A:191:ASP:OD1	2.51	0.44
1:A:6:GLU:O	1:A:7:GLU:OE1	2.36	0.43
1:A:258:GLU:OE2	4:A:604:PG4:H11	2.18	0.43
1:A:304:GLN:N	1:A:305:PRO:CD	2.82	0.43
1:B:111:ALA:HA	1:B:123:ARG:O	2.18	0.43
1:B:344:LYS:HD3	1:B:344:LYS:HA	1.88	0.43
1:B:410:PHE:CB	1:B:433:THR:HG21	2.49	0.42
1:B:151:VAL:O	1:B:201:TYR:HA	2.19	0.42
1:B:368:THR:O	1:B:369:LEU:HG	2.19	0.42
1:A:231:GLN:HE21	1:A:231:GLN:HA	1.85	0.42
1:B:126:LEU:C	1:B:126:LEU:HD23	2.40	0.42
1:B:158:GLN:HE21	1:B:158:GLN:HB3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ILE:HD12	1:A:519:ILE:N	2.35	0.41
1:B:304:GLN:N	1:B:305:PRO:CD	2.83	0.41
1:A:6:GLU:C	1:A:7:GLU:OE1	2.57	0.41
1:A:69:VAL:HG13	1:A:69:VAL:O	2.21	0.41
1:B:401:LEU:C	1:B:401:LEU:HD23	2.40	0.41
1:A:151:VAL:O	1:A:201:TYR:HA	2.20	0.41
1:A:7:GLU:OE1	1:A:7:GLU:CA	2.68	0.41
1:B:508:LEU:C	1:B:508:LEU:HD23	2.41	0.41
1:B:369:LEU:C	1:B:369:LEU:HD12	2.42	0.40
1:A:307:TYR:HB3	1:A:308:PRO:HD3	2.03	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	525/552 (95%)	508 (97%)	16 (3%)	1 (0%)	47	68
1	B	519/552 (94%)	499 (96%)	16 (3%)	4 (1%)	19	35
All	All	1044/1104 (95%)	1007 (96%)	32 (3%)	5 (0%)	29	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	41	GLY
1	B	146	ALA
1	B	172	ILE
1	B	117	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	462/476 (97%)	442 (96%)	20 (4%)	29 53
1	B	459/476 (96%)	431 (94%)	28 (6%)	18 36
All	All	921/952 (97%)	873 (95%)	48 (5%)	24 44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	GLU
1	A	16	LEU
1	A	31	SER
1	A	33	GLU
1	A	69	VAL
1	A	87	SER
1	A	134	ASP
1	A	191	ASP
1	A	196	LEU
1	A	212	PRO
1	A	272	THR
1	A	297	LEU
1	A	318	ASP
1	A	342	GLN
1	A	344	LYS
1	A	369	LEU
1	A	516[A]	ASP
1	A	516[B]	ASP
1	A	547	ASN
1	B	16	LEU
1	B	31	SER
1	B	33	GLU
1	B	87	SER
1	B	118	ASP
1	B	119	THR
1	B	134	ASP

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Mol	Chain	Res	Type
1	B	173	GLU
1	B	191	ASP
1	B	212	PRO
1	B	229	ARG
1	B	264	ILE
1	B	270	GLN
1	B	298	LYS
1	B	318	ASP
1	B	342	GLN
1	B	344	LYS
1	B	352	LYS
1	B	367	ILE
1	B	369	LEU
1	B	390	LEU
1	B	426	THR
1	B	432	THR
1	B	433	THR
1	B	469	SER
1	B	491	THR
1	B	507	GLU
1	B	547	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	185	GLN
1	A	231	GLN
1	A	464	HIS
1	A	488	ASN
1	A	532	ASN
1	B	95	GLN
1	B	158	GLN
1	B	186	ASN
1	B	231	GLN
1	B	488	ASN
1	B	532	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CRF	B	66	1	25,26,27	3.34	9 (36%)	32,37,39	3.84	13 (40%)
1	CR2	A	448	1	20,20,21	3.71	7 (35%)	25,27,29	4.37	12 (48%)
1	CR2	B	448	1	20,20,21	4.16	6 (30%)	25,27,29	3.89	13 (52%)
1	CRF	A	66	1	25,26,27	3.25	8 (32%)	32,37,39	4.12	13 (40%)

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
1	CRF	B	66	1	-	0/10/31/32	0/3/3/3
1	CR2	A	448	1	-	0/6/25/26	0/2/2/2
1	CR2	B	448	1	-	0/6/25/26	0/2/2/2
1	CRF	A	66	1	-	0/10/31/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	448	CR2	CB2-CA2	16.61	1.49	1.35
1	A	448	CR2	CB2-CA2	14.06	1.46	1.35
1	B	66	CRF	CB2-CA2	13.61	1.46	1.35
1	A	66	CRF	CB2-CA2	13.50	1.46	1.35
1	B	448	CR2	C1-N2	4.34	1.40	1.32
1	A	66	CRF	C1-N2	4.15	1.38	1.32
1	A	448	CR2	CD1-CG2	-4.11	1.31	1.39
1	B	66	CRF	C1-N2	4.06	1.38	1.32
1	B	448	CR2	O2-C2	3.79	1.31	1.23
1	B	66	CRF	O2-C2	3.76	1.31	1.23
1	A	66	CRF	CE3-CD2	-3.67	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	CR2	C2-N3	-3.57	1.31	1.39
1	B	66	CRF	CZ3-CE3	3.38	1.44	1.36
1	A	448	CR2	C1-N2	3.25	1.38	1.32
1	B	66	CRF	CA3-N3	-3.17	1.41	1.47
1	A	448	CR2	CA2-N2	-3.07	1.32	1.38
1	B	448	CR2	CE1-CZ	2.88	1.44	1.38
1	A	66	CRF	CH2-CZ2	2.78	1.43	1.36
1	B	448	CR2	OH-CZ	2.70	1.43	1.37
1	A	448	CR2	OH-CZ	2.58	1.43	1.37
1	B	66	CRF	C2-N3	-2.56	1.33	1.39
1	A	66	CRF	O2-C2	2.56	1.28	1.23
1	A	66	CRF	C2-N3	-2.51	1.34	1.39
1	B	66	CRF	CA1-C1	-2.48	1.47	1.51
1	A	66	CRF	CG2-CD2	2.44	1.47	1.41
1	B	448	CR2	C2-N3	-2.36	1.34	1.39
1	B	66	CRF	CH2-CZ2	2.25	1.41	1.36
1	B	66	CRF	CA2-C2	-2.15	1.46	1.48
1	A	448	CR2	CE2-CD2	-2.13	1.34	1.38
1	A	66	CRF	C1-N3	2.10	1.40	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	448	CR2	CA2-C2-N3	16.21	111.04	103.37
1	A	66	CRF	O2-C2-CA2	-14.31	122.92	130.96
1	B	66	CRF	CA2-C2-N3	14.03	110.00	103.37
1	A	66	CRF	CA2-C2-N3	12.93	109.48	103.37
1	B	448	CR2	O2-C2-CA2	-11.55	124.48	130.96
1	B	448	CR2	CA2-C2-N3	10.33	108.25	103.37
1	B	66	CRF	O2-C2-CA2	-9.98	125.36	130.96
1	A	448	CR2	C2-N3-C1	-9.07	103.56	107.99
1	A	66	CRF	C2-N3-C1	-6.59	104.63	107.97
1	B	66	CRF	C2-N3-C1	-6.01	104.92	107.97
1	B	448	CR2	O3-C3-CA3	-6.00	108.27	126.39
1	B	448	CR2	C2-N3-C1	-5.78	105.17	107.99
1	A	66	CRF	CG2-CB2-CA2	-5.03	121.06	130.81
1	A	448	CR2	CD1-CE1-CZ	4.96	125.31	119.88
1	A	448	CR2	O2-C2-CA2	-4.71	128.31	130.96
1	B	66	CRF	C2-CA2-N2	-4.65	105.67	108.93
1	B	66	CRF	CG2-CB2-CA2	-4.32	122.43	130.81
1	A	448	CR2	C2-CA2-N2	-4.29	105.92	108.93
1	B	66	CRF	CB2-CA2-C2	3.98	127.03	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CRF	OG1-CB1-CA1	3.97	117.53	109.04
1	A	66	CRF	CE3-CD2-CE2	3.91	123.35	118.17
1	A	66	CRF	CB2-CA2-C2	3.53	126.49	122.28
1	B	66	CRF	CA1-C1-N3	-3.47	120.59	124.75
1	B	66	CRF	CA3-N3-C1	3.43	131.28	127.16
1	A	448	CR2	CB2-CA2-C2	3.39	126.32	122.28
1	A	448	CR2	O3-C3-CA3	-3.34	116.32	126.39
1	A	66	CRF	N3-C1-N2	3.30	113.74	111.45
1	A	66	CRF	C2-CA2-N2	-3.29	106.63	108.93
1	B	448	CR2	C1-CA1-N1	-3.13	105.92	112.85
1	A	66	CRF	OG1-CB1-CA1	3.01	115.48	109.04
1	A	66	CRF	O3-C3-CA3	-2.88	117.70	126.39
1	A	448	CR2	CE2-CD2-CG2	2.85	124.97	121.25
1	B	448	CR2	CD1-CE1-CZ	2.74	122.88	119.88
1	B	66	CRF	O3-C3-CA3	-2.72	118.19	126.39
1	B	448	CR2	CE2-CZ-CE1	-2.71	115.19	119.77
1	B	448	CR2	N3-C1-N2	2.59	114.86	111.76
1	A	448	CR2	CE1-CD1-CG2	-2.57	117.90	121.25
1	B	66	CRF	C1-CA1-N1	-2.57	105.80	109.96
1	A	66	CRF	CZ3-CE3-CD2	-2.45	117.50	120.89
1	A	448	CR2	C1-CA1-N1	-2.41	107.52	112.85
1	A	448	CR2	CA3-N3-C1	2.39	131.15	127.86
1	B	448	CR2	CG2-CB2-CA2	-2.25	127.18	129.94
1	B	66	CRF	CE3-CD2-CE2	2.24	121.14	118.17
1	B	448	CR2	CA3-N3-C1	2.23	130.93	127.86
1	B	448	CR2	CD2-CE2-CZ	2.22	122.31	119.88
1	B	66	CRF	N3-C1-N2	2.21	112.98	111.45
1	A	66	CRF	CG1-CB1-CA1	-2.21	106.96	112.16
1	B	448	CR2	OH-CZ-CE1	2.18	126.23	120.02
1	A	66	CRF	CA1-C1-N3	-2.15	122.17	124.75
1	A	448	CR2	O2-C2-N3	-2.13	120.12	124.35
1	B	448	CR2	CD2-CG2-CB2	-2.01	114.37	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRF	3	0
1	B	448	CR2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRF	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	GOL	B	603	-	5,5,5	0.46	0	5,5,5	0.84	0
4	PG4	A	605	-	3,3,12	0.80	0	2,2,11	0.24	0
5	FMT	A	606	-	2,2,2	0.91	0	1,1,1	0.67	0
3	GOL	B	604	-	5,5,5	0.41	0	5,5,5	0.79	0
5	FMT	B	606	-	2,2,2	0.82	0	1,1,1	0.80	0
5	FMT	B	607	-	2,2,2	1.11	0	1,1,1	0.54	0
3	GOL	A	603	-	5,5,5	0.69	0	5,5,5	0.72	0
4	PG4	A	604	-	3,3,12	0.65	0	2,2,11	0.87	0
5	FMT	B	605	-	2,2,2	1.27	0	1,1,1	0.19	0
5	FMT	A	607	-	2,2,2	1.14	0	1,1,1	0.41	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	B	603	-	-	2/4/4/4	-
4	PG4	A	605	-	-	1/1/1/10	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	604	-	-	1/1/1/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	C1-C2-C3-O3
3	B	603	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
3	B	604	GOL	O1-C1-C2-O2
4	A	605	PG4	O4-C7-C8-O5
3	A	603	GOL	O2-C2-C3-O3
3	B	603	GOL	O2-C2-C3-O3
4	A	604	PG4	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	PG4	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	530/552 (96%)	-0.19	4 (0%)	86	87	36, 61, 95, 123	0
1	B	528/552 (95%)	-0.10	6 (1%)	80	82	38, 65, 100, 123	0
All	All	1058/1104 (95%)	-0.15	10 (0%)	84	86	36, 63, 97, 123	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	2.7
1	B	13	VAL	2.7
1	A	16	LEU	2.4
1	B	398	LEU	2.3
1	A	118	ASP	2.3
1	B	118	ASP	2.2
1	B	371	MET	2.2
1	A	11	GLY	2.2
1	B	12	VAL	2.1
1	A	115	PHE	2.1

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

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
1	CRF	A	66	24/25	0.97	0.14	51,56,65,71	0
1	CRF	B	66	24/25	0.98	0.15	40,43,56,58	0
1	CR2	B	448	19/20	0.98	0.13	43,46,51,53	0
1	CR2	A	448	19/20	0.99	0.13	37,39,44,45	0

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
4	PG4	A	604	4/13	0.84	0.18	59,68,70,74	0
3	GOL	B	604	6/6	0.85	0.17	74,81,84,85	0
5	FMT	A	606	3/3	0.86	0.13	70,70,74,76	0
5	FMT	A	607	3/3	0.87	0.14	57,57,75,76	0
3	GOL	A	603	6/6	0.89	0.22	56,59,65,67	0
5	FMT	B	606	3/3	0.89	0.14	65,65,72,73	0
2	CA	B	602	1/1	0.90	0.07	68,68,68,68	0
5	FMT	B	605	3/3	0.91	0.24	59,59,68,78	0
2	CA	A	602	1/1	0.91	0.07	64,64,64,64	0
5	FMT	B	607	3/3	0.91	0.35	53,53,84,84	0
4	PG4	A	605	4/13	0.93	0.16	45,58,63,63	0
2	CA	B	601	1/1	0.93	0.09	52,52,52,52	0
3	GOL	B	603	6/6	0.95	0.18	51,60,67,68	0
2	CA	A	601	1/1	0.97	0.08	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.