Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 06:34 PM JST

PDB ID	:	6LXT
Title	:	Structure of post fusion core of 2019-nCoV S2 subunit
Authors	:	Zhu, Y.; Sun, F.
Deposited on	:	2020-02-11
Resolution	:	2.90 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:

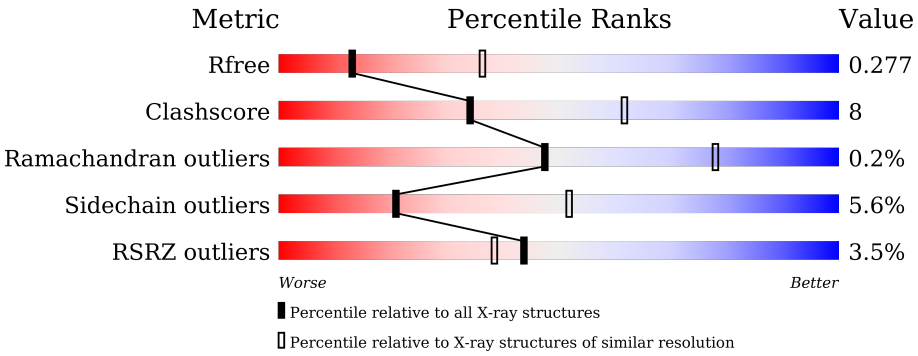
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	132	2% 72% 14% • 12%
1	B	132	2% 73% 13% • 12%
1	C	132	2% 77% 12% 11%
1	D	132	4% 69% 14% • 17%
1	E	132	7% 76% 11% 14%
1	F	132	2% 70% 14% • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG4	A	1303	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5237 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 Spike protein S2, Spike protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	116	Total 881	C 543	N 153	O 185	0	0	0
1	B	116	Total 880	C 543	N 152	O 185	0	0	0
1	C	117	Total 889	C 547	N 154	O 188	0	0	0
1	D	110	Total 831	C 511	N 146	O 174	0	0	0
1	E	114	Total 865	C 534	N 149	O 182	0	0	0
1	F	113	Total 859	C 530	N 150	O 179	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1156	SER	-	linker	UNP P0DTC2
A	1157	GLY	-	linker	UNP P0DTC2
A	1158	GLY	-	linker	UNP P0DTC2
A	1159	ARG	-	linker	UNP P0DTC2
A	1160	GLY	-	linker	UNP P0DTC2
A	1161	GLY	-	linker	UNP P0DTC2
A	1207	GLY	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
B	1156	SER	-	linker	UNP P0DTC2
B	1157	GLY	-	linker	UNP P0DTC2
B	1158	GLY	-	linker	UNP P0DTC2
B	1159	ARG	-	linker	UNP P0DTC2
B	1160	GLY	-	linker	UNP P0DTC2
B	1161	GLY	-	linker	UNP P0DTC2
B	1207	GLY	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
C	1156	SER	-	linker	UNP P0DTC2

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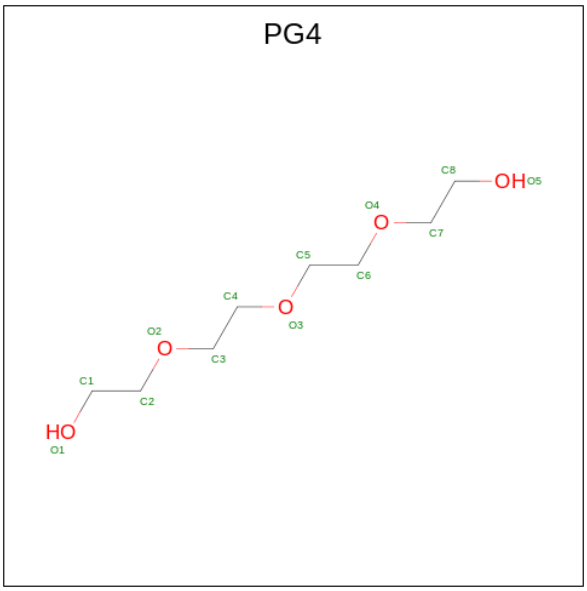
Chain	Residue	Modelled	Actual	Comment	Reference
C	1157	GLY	-	linker	UNP P0DTC2
C	1158	GLY	-	linker	UNP P0DTC2
C	1159	ARG	-	linker	UNP P0DTC2
C	1160	GLY	-	linker	UNP P0DTC2
C	1161	GLY	-	linker	UNP P0DTC2
C	1207	GLY	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
D	1156	SER	-	linker	UNP P0DTC2
D	1157	GLY	-	linker	UNP P0DTC2
D	1158	GLY	-	linker	UNP P0DTC2
D	1159	ARG	-	linker	UNP P0DTC2
D	1160	GLY	-	linker	UNP P0DTC2
D	1161	GLY	-	linker	UNP P0DTC2
D	1207	GLY	-	expression tag	UNP P0DTC2
D	1208	GLY	-	expression tag	UNP P0DTC2
E	1156	SER	-	linker	UNP P0DTC2
E	1157	GLY	-	linker	UNP P0DTC2
E	1158	GLY	-	linker	UNP P0DTC2
E	1159	ARG	-	linker	UNP P0DTC2
E	1160	GLY	-	linker	UNP P0DTC2
E	1161	GLY	-	linker	UNP P0DTC2
E	1207	GLY	-	expression tag	UNP P0DTC2
E	1208	GLY	-	expression tag	UNP P0DTC2
F	1156	SER	-	linker	UNP P0DTC2
F	1157	GLY	-	linker	UNP P0DTC2
F	1158	GLY	-	linker	UNP P0DTC2
F	1159	ARG	-	linker	UNP P0DTC2
F	1160	GLY	-	linker	UNP P0DTC2
F	1161	GLY	-	linker	UNP P0DTC2
F	1207	GLY	-	expression tag	UNP P0DTC2
F	1208	GLY	-	expression tag	UNP P0DTC2

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	A	1	Total C O 13 8 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

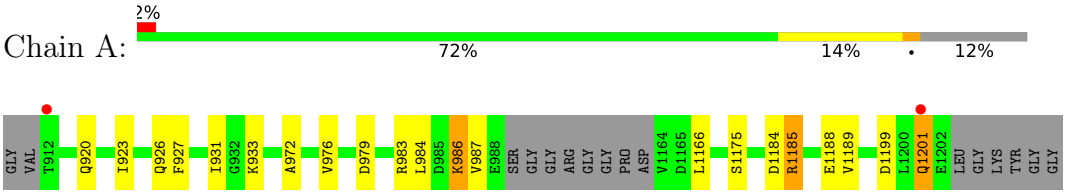
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0

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.

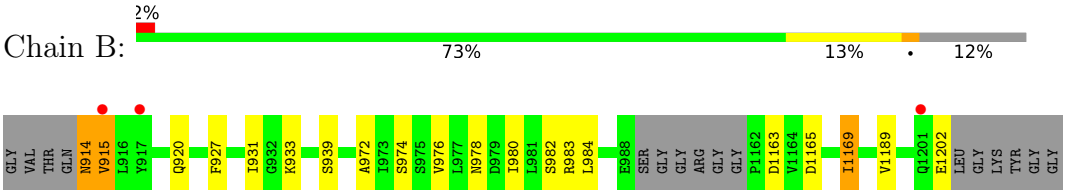
• Molecule 1: Spike protein S2, Spike protein S2

Chain A:



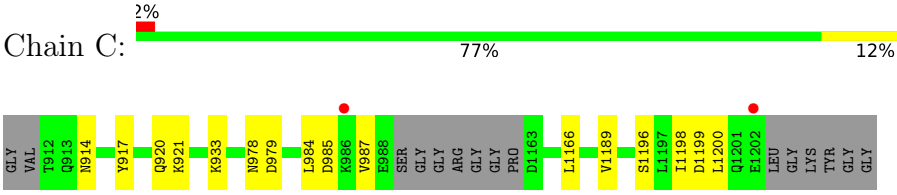
• Molecule 1: Spike protein S2, Spike protein S2

Chain B:



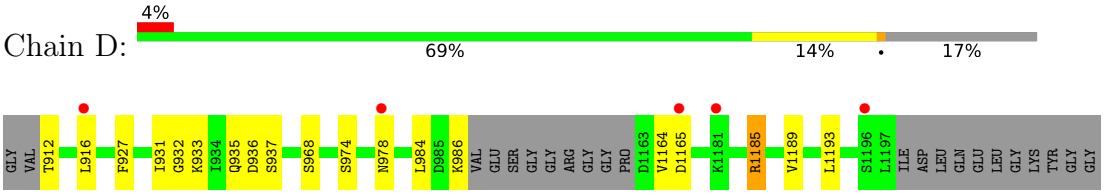
• Molecule 1: Spike protein S2, Spike protein S2

Chain C:



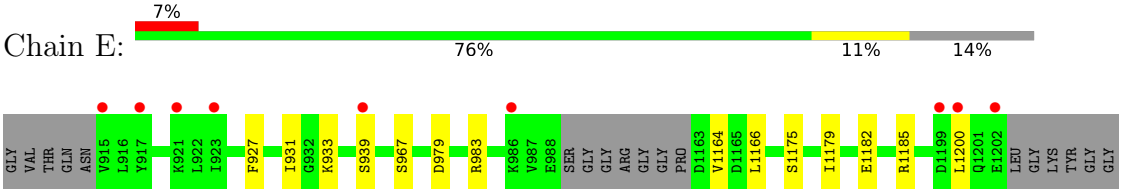
• Molecule 1: Spike protein S2, Spike protein S2

Chain D:



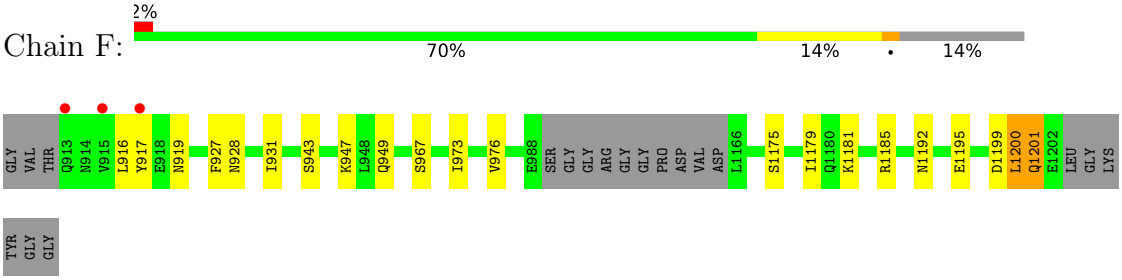
• Molecule 1: Spike protein S2, Spike protein S2

Chain E:



• Molecule 1: Spike protein S2, Spike protein S2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.24Å 57.58Å 115.72Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	47.32 – 2.90 47.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (47.32-2.90) 94.0 (47.32-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.259 , 0.290 0.258 , 0.277	Depositor DCC
R_{free} test set	737 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5237	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.73% 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: PG4, ZN

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	0.69	0/882	0.78	0/1191
1	B	0.67	0/882	0.75	0/1191
1	C	0.69	0/890	0.75	0/1202
1	D	0.70	0/832	0.78	0/1123
1	E	0.70	0/866	0.77	0/1169
1	F	0.69	0/860	0.78	0/1160
All	All	0.69	0/5212	0.77	0/7036

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	881	0	896	26	0
1	B	880	0	893	22	0
1	C	889	0	900	21	0
1	D	831	0	845	23	0
1	E	865	0	879	16	0
1	F	859	0	876	17	0
2	A	26	0	36	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	F	2	0	0	0	0
All	All	5237	0	5325	89	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 8.

All (89) 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:A:1184:ASP:OD2	2:A:1303:PG4:H52	1.51	1.09
1:A:920:GLN:HG2	1:C:920:GLN:HE22	1.25	1.01
1:B:920:GLN:NE2	1:C:920:GLN:HG2	1.85	0.91
1:A:1188:GLU:HG2	2:A:1303:PG4:O1	1.71	0.91
1:B:920:GLN:HE21	1:C:920:GLN:HE21	1.20	0.88
1:D:1185:ARG:HH11	1:D:1185:ARG:HA	1.37	0.86
1:B:927:PHE:CZ	1:B:931:ILE:HD11	2.14	0.83
1:A:1184:ASP:OD1	2:A:1303:PG4:C6	2.31	0.78
1:A:983:ARG:HD2	1:C:984:LEU:HD23	1.64	0.78
1:F:927:PHE:CZ	1:F:931:ILE:HD11	2.19	0.77
2:A:1303:PG4:O5	2:A:1303:PG4:H42	1.85	0.76
1:D:927:PHE:CZ	1:D:931:ILE:HD11	2.21	0.76
1:A:927:PHE:CZ	1:A:931:ILE:HD11	2.21	0.75
1:A:1184:ASP:OD1	2:A:1303:PG4:H62	1.86	0.75
1:E:927:PHE:CZ	1:E:931:ILE:HD11	2.23	0.74
1:D:1189:VAL:HG13	1:E:933:LYS:HB3	1.70	0.73
1:A:920:GLN:CG	1:C:920:GLN:HE22	2.00	0.71
1:D:984:LEU:HD21	1:E:983:ARG:HB3	1.71	0.71
1:B:920:GLN:HE22	1:C:920:GLN:HG2	1.56	0.69
1:E:1166:LEU:HD11	1:F:973:ILE:HG13	1.73	0.69
1:A:1184:ASP:CG	2:A:1303:PG4:H52	2.14	0.67
1:D:1185:ARG:HH11	1:D:1185:ARG:CA	2.08	0.67
1:D:912:THR:HB	1:F:917:TYR:OH	1.95	0.66
1:D:984:LEU:HD21	1:E:983:ARG:HD3	1.79	0.65
1:D:984:LEU:CD2	1:E:983:ARG:HD3	2.26	0.64
1:D:933:LYS:NZ	1:F:1192:ASN:O	2.31	0.63
2:A:1303:PG4:C4	2:A:1303:PG4:C8	2.75	0.63
1:D:984:LEU:HD21	1:E:983:ARG:CB	2.29	0.61
2:A:1303:PG4:C4	2:A:1303:PG4:H82	2.31	0.60
1:B:1189:VAL:HG13	1:C:933:LYS:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HD21	1:B:983:ARG:HD3	1.84	0.59
1:B:920:GLN:HE21	1:C:920:GLN:HG2	1.68	0.58
1:D:984:LEU:HD21	1:E:983:ARG:CD	2.33	0.58
1:A:920:GLN:HG2	1:C:920:GLN:NE2	2.09	0.56
1:B:984:LEU:HD11	1:C:984:LEU:HD12	1.87	0.56
1:D:932:GLY:HA2	1:D:935:GLN:HE21	1.70	0.56
1:E:1182:GLU:OE1	1:F:943:SER:HB3	2.05	0.56
1:A:1188:GLU:CG	2:A:1303:PG4:O1	2.47	0.56
1:A:933:LYS:HB3	1:C:1189:VAL:HG13	1.89	0.55
1:E:1164:VAL:CG1	1:F:976:VAL:HG21	2.36	0.55
1:A:984:LEU:HD11	1:B:983:ARG:HD3	1.88	0.55
1:C:1200:LEU:H	1:C:1200:LEU:HD12	1.72	0.54
1:D:984:LEU:HD23	1:D:984:LEU:O	2.07	0.54
1:D:1185:ARG:HA	1:D:1185:ARG:NH1	2.15	0.54
1:D:974:SER:HB2	1:D:1164:VAL:HG11	1.90	0.53
2:A:1303:PG4:O5	2:A:1303:PG4:C4	2.54	0.53
1:F:949:GLN:NE2	1:F:1179:ILE:H	2.07	0.52
1:E:1179:ILE:HG22	1:F:947:LYS:HD2	1.92	0.52
1:A:984:LEU:HD11	1:B:983:ARG:CB	2.40	0.52
1:D:1193:LEU:HD23	1:E:933:LYS:HD2	1.92	0.52
1:B:920:GLN:HE21	1:C:920:GLN:NE2	1.97	0.51
1:C:1200:LEU:HD12	1:C:1200:LEU:N	2.26	0.51
1:D:916:LEU:HD13	1:F:916:LEU:HD13	1.92	0.51
1:A:984:LEU:CD2	1:B:983:ARG:HD3	2.41	0.50
1:A:984:LEU:HD11	1:B:983:ARG:HB3	1.94	0.49
2:A:1303:PG4:H82	2:A:1303:PG4:H41	1.94	0.49
2:A:1303:PG4:O3	2:A:1303:PG4:C2	2.60	0.48
1:C:1200:LEU:H	1:C:1200:LEU:CD1	2.26	0.48
1:E:1164:VAL:HG11	1:F:976:VAL:HG21	1.94	0.48
1:A:1201:GLN:HE21	1:B:915:VAL:HG22	1.77	0.48
1:D:936:ASP:HB3	1:F:1185:ARG:HH21	1.79	0.48
1:D:978:ASN:OD1	1:D:1164:VAL:HG23	2.13	0.47
1:D:984:LEU:CD2	1:E:983:ARG:CD	2.92	0.47
1:E:1200:LEU:HD12	1:F:919:ASN:CG	2.35	0.47
1:D:1185:ARG:NH1	1:D:1185:ARG:HG2	2.29	0.47
1:B:980:ILE:O	1:B:984:LEU:HD23	2.15	0.47
1:B:974:SER:O	1:B:978:ASN:ND2	2.47	0.47
1:A:926:GLN:HB3	1:C:1196:SER:O	2.15	0.46
1:D:1185:ARG:HH11	1:D:1185:ARG:CG	2.28	0.46
1:A:987:VAL:HG11	1:C:987:VAL:HG11	1.96	0.46
1:A:972:ALA:O	1:A:976:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1199:ASP:C	1:F:1201:GLN:H	2.18	0.46
1:A:984:LEU:CD1	1:B:983:ARG:HD3	2.46	0.46
1:B:972:ALA:O	1:B:976:VAL:HG23	2.15	0.46
2:A:1303:PG4:O3	2:A:1303:PG4:H22	2.17	0.45
1:A:923:ILE:HG12	1:C:1198:ILE:HD13	1.97	0.45
1:B:920:GLN:NE2	1:C:920:GLN:HE21	2.01	0.45
1:C:917:TYR:CE2	1:C:921:LYS:HE3	2.51	0.45
1:B:914:ASN:N	1:B:914:ASN:OD1	2.50	0.44
1:F:928:ASN:ND2	1:F:1200:LEU:CD2	2.81	0.43
1:A:986:LYS:HA	1:A:986:LYS:HD3	1.73	0.43
1:B:1169:ILE:H	1:B:1169:ILE:HD13	1.84	0.43
1:F:1199:ASP:O	1:F:1201:GLN:N	2.52	0.42
1:A:1185:ARG:NH1	2:A:1301:PG4:H32	2.34	0.42
1:A:1189:VAL:HG13	1:B:933:LYS:HB3	2.03	0.41
1:E:1164:VAL:HG13	1:F:976:VAL:HG21	2.01	0.41
1:C:978:ASN:HD22	1:C:978:ASN:HA	1.78	0.41
1:F:1195:GLU:O	1:F:1195:GLU:HG3	2.21	0.40
1:D:932:GLY:HA2	1:D:935:GLN:NE2	2.36	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	112/132 (85%)	112 (100%)	0	0	100	100
1	B	112/132 (85%)	112 (100%)	0	0	100	100
1	C	113/132 (86%)	110 (97%)	3 (3%)	0	100	100
1	D	106/132 (80%)	104 (98%)	2 (2%)	0	100	100
1	E	110/132 (83%)	108 (98%)	2 (2%)	0	100	100
1	F	109/132 (83%)	102 (94%)	6 (6%)	1 (1%)	17	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	662/792 (84%)	648 (98%)	13 (2%)	1 (0%)	47 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1200	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	102/110 (93%)	95 (93%)	7 (7%)	15 41
1	B	102/110 (93%)	94 (92%)	8 (8%)	12 34
1	C	103/110 (94%)	98 (95%)	5 (5%)	25 57
1	D	96/110 (87%)	91 (95%)	5 (5%)	23 55
1	E	100/110 (91%)	95 (95%)	5 (5%)	24 57
1	F	99/110 (90%)	95 (96%)	4 (4%)	31 65
All	All	602/660 (91%)	568 (94%)	34 (6%)	21 52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	979	ASP
1	A	986	LYS
1	A	1166	LEU
1	A	1175	SER
1	A	1185	ARG
1	A	1199	ASP
1	A	1201	GLN
1	B	914	ASN
1	B	915	VAL
1	B	939	SER
1	B	982	SER

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Mol	Chain	Res	Type
1	B	1163	ASP
1	B	1165	ASP
1	B	1169	ILE
1	B	1202	GLU
1	C	914	ASN
1	C	979	ASP
1	C	985	ASP
1	C	1166	LEU
1	C	1199	ASP
1	D	937	SER
1	D	968	SER
1	D	986	LYS
1	D	1165	ASP
1	D	1185	ARG
1	E	939	SER
1	E	967	SER
1	E	979	ASP
1	E	1175	SER
1	E	1185	ARG
1	F	967	SER
1	F	1175	SER
1	F	1181	LYS
1	F	1201	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	949	GLN
1	A	1201	GLN
1	B	914	ASN
1	B	949	GLN
1	B	957	GLN
1	B	1187	ASN
1	C	914	ASN
1	C	920	GLN
1	C	935	GLN
1	C	949	GLN
1	C	978	ASN
1	C	1187	ASN
1	C	1201	GLN
1	D	926	GLN
1	D	935	GLN

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Mol	Chain	Res	Type
1	D	949	GLN
1	F	926	GLN
1	F	935	GLN
1	F	949	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	PG4	A	1303	-	12,12,12	0.46	0	11,11,11	1.61	3 (27%)
2	PG4	A	1301	-	12,12,12	0.73	0	11,11,11	0.94	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
2	PG4	A	1303	-	-	6/10/10/10	-
2	PG4	A	1301	-	-	5/10/10/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1303	PG4	O2-C3-C4	-3.52	94.53	110.39
2	A	1303	PG4	O5-C8-C7	-2.01	100.14	111.81
2	A	1303	PG4	O4-C7-C8	2.00	118.87	110.07

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	PG4	O3-C5-C6-O4
2	A	1303	PG4	O4-C7-C8-O5
2	A	1303	PG4	O1-C1-C2-O2
2	A	1301	PG4	O2-C3-C4-O3
2	A	1301	PG4	O1-C1-C2-O2
2	A	1303	PG4	C5-C6-O4-C7
2	A	1303	PG4	C8-C7-O4-C6
2	A	1303	PG4	O3-C5-C6-O4
2	A	1301	PG4	C6-C5-O3-C4
2	A	1303	PG4	C1-C2-O2-C3
2	A	1301	PG4	C8-C7-O4-C6

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1303	PG4	13	0
2	A	1301	PG4	1	0

5.7 Other polymers

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	116/132 (87%)	0.02	2 (1%)	70	69	49, 75, 124, 142	0
1	B	116/132 (87%)	0.01	3 (2%)	56	52	42, 72, 114, 124	0
1	C	117/132 (88%)	-0.01	2 (1%)	70	69	49, 71, 119, 148	0
1	D	110/132 (83%)	0.18	5 (4%)	33	29	68, 97, 137, 142	0
1	E	114/132 (86%)	0.43	9 (7%)	12	10	67, 98, 143, 155	0
1	F	113/132 (85%)	-0.04	3 (2%)	54	50	48, 82, 124, 135	0
All	All	686/792 (86%)	0.10	24 (3%)	44	38	42, 84, 129, 155	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	912	THR	6.2
1	E	939	SER	3.8
1	D	1196	SER	3.5
1	E	1202	GLU	3.5
1	D	1165	ASP	3.4
1	C	1202	GLU	3.3
1	E	915	VAL	3.3
1	E	921	LYS	3.0
1	E	923	ILE	2.8
1	F	915	VAL	2.5
1	B	1201	GLN	2.4
1	B	917	TYR	2.4
1	E	1200	LEU	2.4
1	E	917	TYR	2.4
1	D	916	LEU	2.4
1	C	986	LYS	2.3
1	B	915	VAL	2.3
1	D	978	ASN	2.2
1	A	1201	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1181	LYS	2.1
1	E	986	LYS	2.1
1	E	1199	ASP	2.1
1	F	913	GLN	2.1
1	F	917	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZN	A	1302	1/1	0.63	0.21	150,150,150,150	0
3	ZN	F	1301	1/1	0.79	0.07	148,148,148,148	0
2	PG4	A	1301	13/13	0.82	0.20	54,67,84,84	0
3	ZN	A	1304	1/1	0.88	0.15	117,117,117,117	0
2	PG4	A	1303	13/13	0.93	0.32	41,53,83,83	0
3	ZN	F	1302	1/1	0.93	0.12	145,145,145,145	0
3	ZN	B	1302	1/1	0.94	0.07	145,145,145,145	0
3	ZN	B	1301	1/1	0.97	0.13	103,103,103,103	0

6.5 Other polymers (i)

There are no such residues in this entry.