Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:58 AM EDT

PDB ID	:	2PYF
Title	:	Crystal Structures of High Affinity Human T-Cell Receptors Bound to pMHC RevealNative Diagonal Binding Geometry Unbound TCR Clone 5-1
Authors	:	Sami, M.; Rizkallah, P.J.; Dunn, S.; Li, Y.; Moysey, R.; Vuidepot, A.; Baston, E.; Todorov, P.; Molloy, P.; Gao, F.; Boulter, J.M.; Jakobsen, B.K.
Deposited on	:	2007-05-16
Resolution	:	2.20 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:

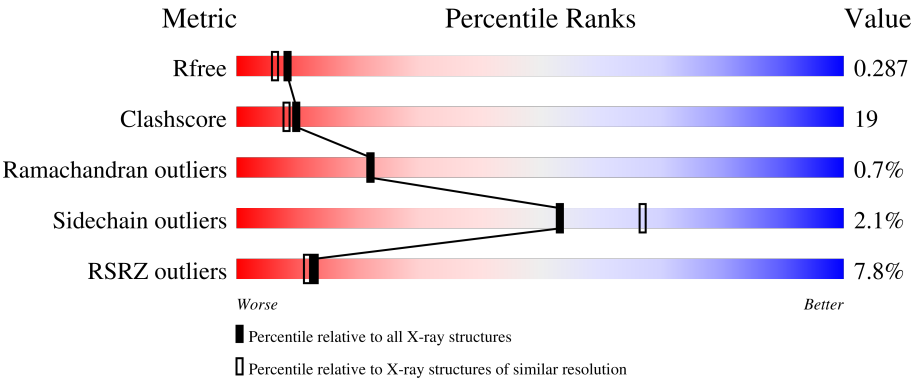
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	205	12% 67% 31% .
2	B	241	4% 79% 19% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3731 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.

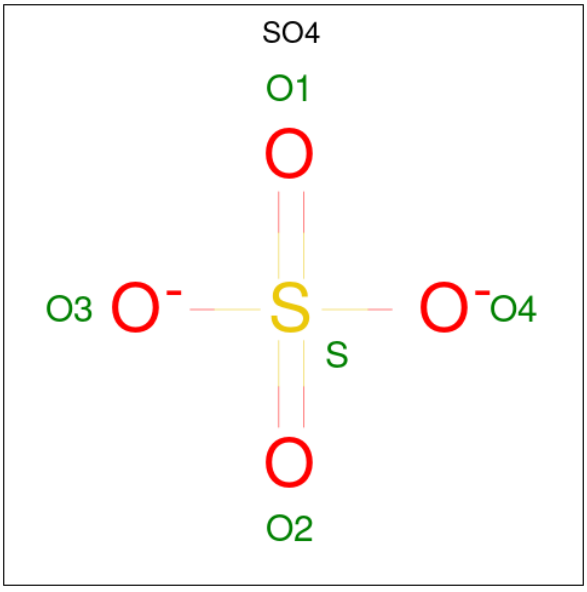
- Molecule 1 is a protein called T-Cell Receptor, Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1584	988	264	325	7			

- Molecule 2 is a protein called T-Cell Receptor, Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1902	1197	327	369	9			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



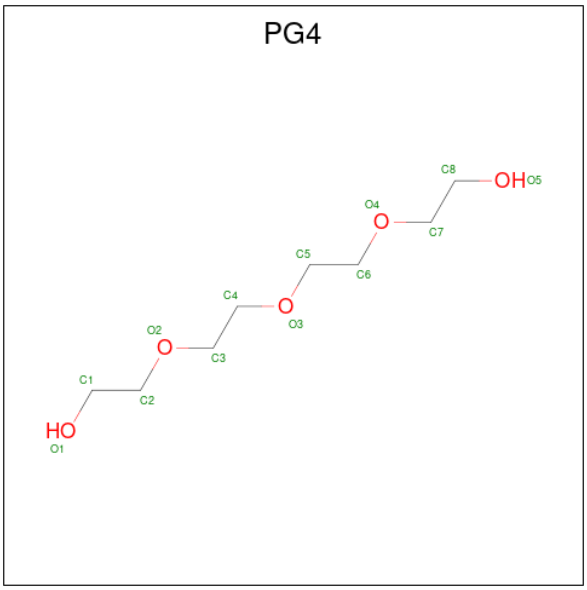
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

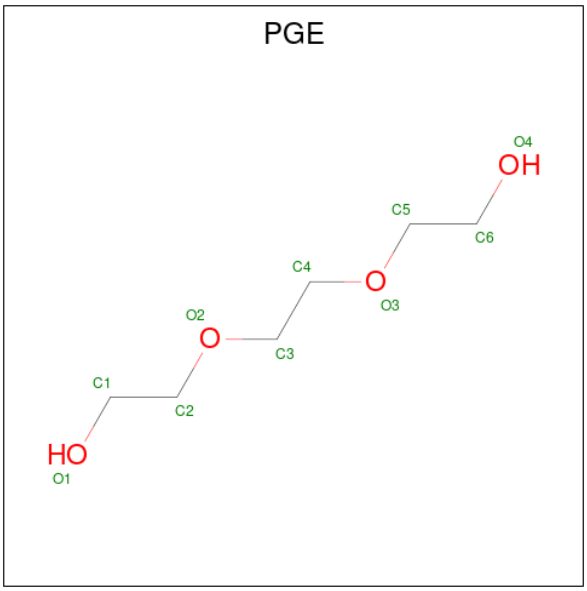
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- 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 13 8 5	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0

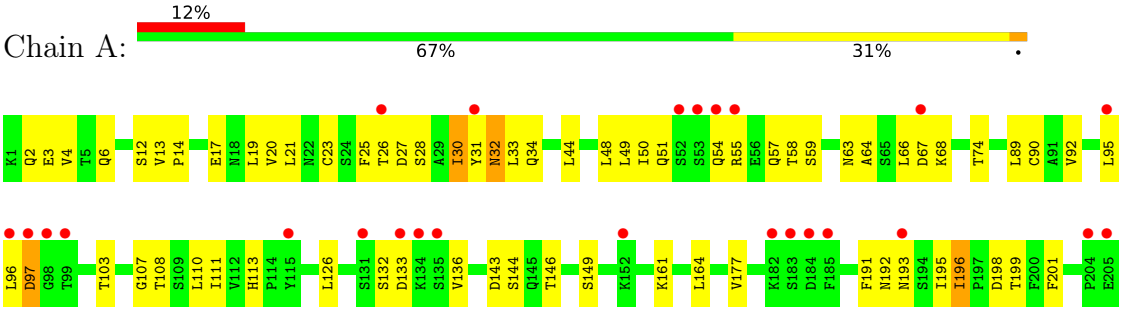
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 79 79	0	1
6	B	82	Total O 83 83	0	1

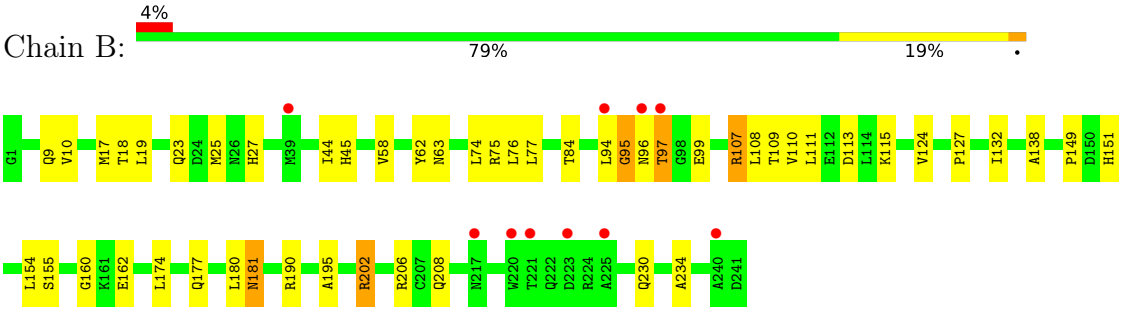
3 Residue-property plots (i)

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: T-Cell Receptor, Alpha Chain



• Molecule 2: T-Cell Receptor, Beta Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.96Å 59.80Å 81.80Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 97.0 (29.90-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.295 0.208 , 0.287	Depositor DCC
R_{free} test set	1064 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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, SO4, PG4

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	0.74	0/1617	0.57	0/2199
2	B	0.83	0/1953	0.65	1/2660 (0.0%)
All	All	0.79	0/3570	0.61	1/4859 (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	B	95	GLY	N-CA-C	-5.39	99.62	113.10

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	1584	0	1522	78	0
2	B	1902	0	1801	60	0
3	A	10	0	0	0	0
3	B	20	0	0	1	0
4	A	13	0	18	3	0
5	A	20	0	28	0	0
5	B	20	0	28	3	0
6	A	79	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	83	0	0	2	0
All	All	3731	0	3397	134	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 19.

All (134) 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:13:VAL:HG11	1:A:19:LEU:HD21	1.54	0.87
1:A:196:ILE:HD12	1:A:196:ILE:H	1.39	0.86
1:A:196:ILE:HD12	1:A:196:ILE:N	1.96	0.81
1:A:4:VAL:HG12	1:A:103:THR:HG22	1.61	0.81
2:B:107:ARG:HH11	2:B:107:ARG:HG3	1.51	0.76
2:B:107:ARG:HH11	2:B:107:ARG:CG	2.00	0.75
1:A:51:GLN:HE22	2:B:97:THR:HA	1.53	0.72
1:A:196:ILE:H	1:A:196:ILE:CD1	2.03	0.72
1:A:33:LEU:HD23	1:A:92:VAL:HG12	1.71	0.70
2:B:202:ARG:CG	2:B:202:ARG:HH21	2.04	0.70
1:A:199:THR:HG23	1:A:201:PHE:CE2	2.28	0.68
2:B:162:GLU:N	3:B:242:SO4:O3	2.26	0.68
1:A:164:LEU:HD12	1:A:164:LEU:O	1.94	0.68
2:B:10:VAL:HG23	6:B:305:HOH:O	1.94	0.66
1:A:49:LEU:C	1:A:49:LEU:HD23	2.16	0.66
1:A:6:GLN:HE22	1:A:89:LEU:HA	1.61	0.66
1:A:51:GLN:HB2	1:A:54:GLN:HG2	1.78	0.66
1:A:13:VAL:HG11	1:A:19:LEU:CD2	2.24	0.66
2:B:108:LEU:HD11	2:B:110:VAL:HG23	1.77	0.65
2:B:108:LEU:HD11	2:B:110:VAL:CG2	2.28	0.64
1:A:13:VAL:HG21	1:A:19:LEU:HD21	1.79	0.64
2:B:108:LEU:CD1	2:B:110:VAL:HG23	2.28	0.64
2:B:180:LEU:HD22	2:B:180:LEU:N	2.13	0.64
2:B:17:MET:HE2	2:B:19:LEU:HD23	1.81	0.62
1:A:199:THR:HG23	1:A:201:PHE:HE2	1.64	0.61
2:B:95:GLY:O	2:B:97:THR:HG22	2.00	0.61
2:B:132:ILE:HG23	2:B:195:ALA:HB1	1.83	0.60
2:B:113:ASP:OD1	2:B:115:LYS:HD3	2.02	0.60
2:B:174:LEU:HD12	2:B:174:LEU:O	2.02	0.59
2:B:149:PRO:HG2	2:B:151:HIS:ND1	2.18	0.59
1:A:66:LEU:C	1:A:66:LEU:HD23	2.23	0.59
1:A:196:ILE:N	1:A:196:ILE:CD1	2.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:GLN:HA	5:B:301:PGE:H22	1.84	0.58
1:A:30:ILE:HD13	1:A:30:ILE:H	1.68	0.58
1:A:196:ILE:HG22	1:A:198:ASP:H	1.68	0.58
1:A:48:LEU:HD21	1:A:59:SER:HB2	1.85	0.58
1:A:193[A]:ASN:OD1	1:A:195:ILE:HG23	2.05	0.56
2:B:132:ILE:HG23	2:B:195:ALA:CB	2.36	0.56
1:A:51:GLN:HB2	1:A:54:GLN:CG	2.36	0.55
2:B:109:THR:HG22	2:B:111:LEU:CD1	2.36	0.54
1:A:196:ILE:O	1:A:199:THR:HG22	2.08	0.54
1:A:33:LEU:HD23	1:A:92:VAL:CG1	2.38	0.54
1:A:96:LEU:O	1:A:97:ASP:HB2	2.08	0.54
1:A:58:THR:HG23	1:A:63:ASN:OD1	2.09	0.53
1:A:49:LEU:HD23	1:A:50:ILE:N	2.24	0.53
2:B:202:ARG:HH21	2:B:202:ARG:HG3	1.73	0.53
2:B:9:GLN:HG2	2:B:17:MET:SD	2.50	0.52
1:A:32:ASN:HD22	1:A:32:ASN:C	2.12	0.52
2:B:109:THR:HG22	2:B:111:LEU:HD11	1.91	0.52
1:A:54:GLN:O	1:A:55:ARG:HB3	2.10	0.52
1:A:2:GLN:NE2	1:A:27:ASP:HB3	2.26	0.51
1:A:2:GLN:OE1	1:A:25:PHE:HB2	2.09	0.51
2:B:177:GLN:HB3	2:B:180:LEU:HD23	1.92	0.51
2:B:206:ARG:HB3	5:B:302:PGE:H62	1.93	0.51
2:B:124:VAL:HG23	2:B:234:ALA:HB3	1.93	0.51
1:A:161:LYS:HZ2	4:A:303:PG4:C1	2.23	0.51
2:B:44:ILE:HG22	2:B:45:HIS:CD2	2.46	0.51
2:B:84:THR:HG23	2:B:109:THR:HA	1.92	0.51
1:A:34:GLN:NE2	2:B:99:GLU:HB2	2.26	0.50
1:A:33:LEU:HD13	1:A:34:GLN:N	2.27	0.50
2:B:174:LEU:HD12	2:B:174:LEU:C	2.32	0.50
1:A:66:LEU:HD23	1:A:67:ASP:N	2.26	0.49
1:A:164:LEU:HD12	1:A:164:LEU:C	2.32	0.49
1:A:50:ILE:HD11	1:A:64:ALA:CB	2.41	0.49
2:B:58:VAL:O	2:B:58:VAL:HG23	2.13	0.49
1:A:31:TYR:HA	1:A:95:LEU:HD13	1.94	0.49
1:A:28:SER:HB2	1:A:68:LYS:O	2.14	0.48
2:B:107:ARG:CG	2:B:107:ARG:NH1	2.66	0.48
2:B:17:MET:HG2	2:B:18:THR:N	2.29	0.47
1:A:48:LEU:HD21	1:A:59:SER:CB	2.44	0.47
2:B:202:ARG:HH21	2:B:202:ARG:HG2	1.78	0.47
1:A:13:VAL:CG1	1:A:19:LEU:HD21	2.35	0.47
1:A:126:LEU:HD12	1:A:126:LEU:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:CD2	2:B:96:ASN:HB3	2.50	0.46
1:A:113:HIS:HB3	1:A:144:SER:HB3	1.97	0.46
1:A:149:SER:O	1:A:193[B]:ASN:ND2	2.48	0.46
1:A:58:THR:HG22	1:A:59:SER:N	2.30	0.46
2:B:127:PRO:HB3	2:B:138:ALA:HB1	1.97	0.46
2:B:17:MET:CE	2:B:19:LEU:HD23	2.45	0.46
1:A:31:TYR:CE2	2:B:96:ASN:HB3	2.51	0.46
1:A:199:THR:CG2	1:A:201:PHE:CE2	2.98	0.46
2:B:25:MET:CE	2:B:27:HIS:CE1	2.99	0.46
2:B:127:PRO:CB	2:B:138:ALA:HB1	2.45	0.46
1:A:195:ILE:HD12	1:A:199:THR:HG21	1.98	0.46
1:A:12:SER:HG	1:A:113:HIS:HE2	1.59	0.45
1:A:13:VAL:HG23	1:A:14:PRO:HD2	1.99	0.45
2:B:108:LEU:C	2:B:108:LEU:HD13	2.36	0.45
2:B:206:ARG:NH1	2:B:208:GLN:OE1	2.48	0.45
1:A:4:VAL:CG2	1:A:23:CYS:SG	3.05	0.45
1:A:44:LEU:HD12	1:A:44:LEU:N	2.31	0.45
2:B:96:ASN:O	2:B:97:THR:HB	2.17	0.45
1:A:96:LEU:O	1:A:97:ASP:CB	2.64	0.45
2:B:154:LEU:HD23	2:B:155:SER:N	2.31	0.45
2:B:181:ASN:O	2:B:181:ASN:ND2	2.49	0.45
2:B:17:MET:CE	2:B:19:LEU:CD2	2.94	0.45
2:B:75:ARG:C	2:B:76:LEU:HD12	2.37	0.45
1:A:3:GLU:HG2	1:A:26:THR:CG2	2.46	0.45
1:A:49:LEU:C	1:A:49:LEU:CD2	2.85	0.45
1:A:3:GLU:H	1:A:26:THR:HG22	1.81	0.44
1:A:146:THR:OG1	1:A:196:ILE:HD11	2.17	0.44
2:B:160:GLY:HA2	5:B:302:PGE:H5	1.98	0.44
2:B:77:LEU:HD22	2:B:77:LEU:N	2.32	0.44
1:A:4:VAL:CG1	1:A:103:THR:HG22	2.42	0.44
1:A:48:LEU:HD22	1:A:57:GLN:HG3	1.98	0.44
2:B:17:MET:HE1	2:B:19:LEU:HD21	1.99	0.44
1:A:191:PHE:O	1:A:193[A]:ASN:N	2.49	0.44
2:B:206:ARG:HD2	6:B:328:HOH:O	2.17	0.44
2:B:62:TYR:HB3	2:B:74:LEU:HD11	2.00	0.43
2:B:62:TYR:C	2:B:63:ASN:HD22	2.21	0.43
2:B:180:LEU:N	2:B:180:LEU:CD2	2.79	0.43
2:B:190:ARG:N	2:B:190:ARG:HD2	2.33	0.43
1:A:50:ILE:HD11	1:A:64:ALA:HB1	2.01	0.43
1:A:66:LEU:C	1:A:66:LEU:CD2	2.86	0.43
2:B:202:ARG:HD3	2:B:202:ARG:H	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:OD2	1:A:144:SER:N	2.52	0.43
1:A:21:LEU:HD22	1:A:108:THR:HG21	2.00	0.42
1:A:113:HIS:ND1	4:A:303:PG4:C1	2.83	0.42
1:A:13:VAL:HG23	1:A:17:GLU:OE1	2.18	0.42
1:A:20:VAL:HG13	1:A:74:THR:CG2	2.49	0.42
1:A:3:GLU:HG2	1:A:26:THR:HG21	2.00	0.42
1:A:136:VAL:CG1	1:A:177:VAL:HG13	2.50	0.42
1:A:161:LYS:HZ2	4:A:303:PG4:H11	1.84	0.42
2:B:127:PRO:CG	2:B:138:ALA:HB1	2.50	0.42
2:B:94:LEU:HD23	2:B:94:LEU:HA	1.89	0.42
1:A:89:LEU:HD23	1:A:107:GLY:CA	2.50	0.42
1:A:199:THR:CG2	1:A:201:PHE:HE2	2.29	0.42
1:A:110:LEU:HD12	1:A:111:ILE:H	1.85	0.41
2:B:109:THR:HG22	2:B:111:LEU:HD12	2.03	0.41
2:B:76:LEU:HD12	2:B:76:LEU:N	2.34	0.41
1:A:132:SER:O	1:A:133:ASP:HB3	2.21	0.41
1:A:33:LEU:CD2	1:A:92:VAL:HG12	2.45	0.41
1:A:33:LEU:HD13	1:A:33:LEU:C	2.42	0.40
2:B:9:GLN:HG2	2:B:17:MET:CE	2.51	0.40
1:A:89:LEU:HD23	1:A:107:GLY:HA3	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	204/205 (100%)	186 (91%)	16 (8%)	2 (1%)	15	14
2	B	239/241 (99%)	227 (95%)	11 (5%)	1 (0%)	34	37
All	All	443/446 (99%)	413 (93%)	27 (6%)	3 (1%)	22	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
2	B	97	THR
1	A	192	ASN

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	183/182 (100%)	179 (98%)	4 (2%)	52 65
2	B	208/208 (100%)	204 (98%)	4 (2%)	57 71
All	All	391/390 (100%)	383 (98%)	8 (2%)	53 69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	32	ASN
1	A	90	CYS
1	A	196	ILE
2	B	23	GLN
2	B	107	ARG
2	B	181	ASN
2	B	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	22	ASN
1	A	32	ASN
1	A	51	GLN
1	A	81	GLN
1	A	117	GLN
1	A	125	GLN
1	A	145	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	147	ASN
1	A	189	ASN
2	B	9	GLN
2	B	15	GLN
2	B	23	GLN
2	B	26	ASN
2	B	55	GLN
2	B	60	ASN
2	B	63	ASN
2	B	96	ASN
2	B	134	HIS
2	B	136	GLN
2	B	172	GLN
2	B	177	GLN
2	B	181	ASN

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)

11 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	SO4	B	244	-	4,4,4	0.11	0	6,6,6	0.08	0
3	SO4	B	245	-	4,4,4	0.15	0	6,6,6	0.08	0
4	PG4	A	303	-	12,12,12	0.56	0	11,11,11	0.15	0
5	PGE	A	304	-	9,9,9	0.55	0	8,8,8	0.20	0
3	SO4	A	206	-	4,4,4	0.14	0	6,6,6	0.08	0
5	PGE	A	305	-	9,9,9	0.66	0	8,8,8	0.12	0
3	SO4	B	243	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	207	-	4,4,4	0.18	0	6,6,6	0.07	0
5	PGE	B	302	-	9,9,9	1.08	0	8,8,8	0.27	0
3	SO4	B	242	-	4,4,4	0.23	0	6,6,6	0.06	0
5	PGE	B	301	-	9,9,9	0.92	0	8,8,8	0.43	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
4	PG4	A	303	-	-	5/10/10/10	-
5	PGE	A	304	-	-	4/7/7/7	-
5	PGE	A	305	-	-	4/7/7/7	-
5	PGE	B	302	-	-	3/7/7/7	-
5	PGE	B	301	-	-	6/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	PGE	C1-C2-O2-C3
5	A	304	PGE	O2-C3-C4-O3
4	A	303	PG4	O3-C5-C6-O4
5	A	304	PGE	O1-C1-C2-O2
5	B	302	PGE	O3-C5-C6-O4
5	A	304	PGE	O3-C5-C6-O4
5	A	305	PGE	O1-C1-C2-O2
5	A	305	PGE	O3-C5-C6-O4
5	B	301	PGE	O1-C1-C2-O2
5	B	301	PGE	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	303	PG4	C8-C7-O4-C6
4	A	303	PG4	C5-C6-O4-C7
5	A	304	PGE	C3-C4-O3-C5
4	A	303	PG4	C1-C2-O2-C3
5	B	301	PGE	O3-C5-C6-O4
4	A	303	PG4	O1-C1-C2-O2
5	B	301	PGE	C3-C4-O3-C5
5	B	302	PGE	C4-C3-O2-C2
5	B	302	PGE	O2-C3-C4-O3
5	B	301	PGE	C4-C3-O2-C2
5	A	305	PGE	O2-C3-C4-O3
5	A	305	PGE	C1-C2-O2-C3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	PG4	3	0
5	B	302	PGE	2	0
3	B	242	SO4	1	0
5	B	301	PGE	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	205/205 (100%)	0.59	25 (12%)	4	3	9, 22, 50, 61	0
2	B	241/241 (100%)	0.20	10 (4%)	37	35	4, 17, 36, 55	0
All	All	446/446 (100%)	0.38	35 (7%)	13	11	4, 19, 45, 61	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	SER	6.7
1	A	184	ASP	6.4
2	B	221	THR	6.4
1	A	96	LEU	5.7
1	A	133	ASP	5.1
2	B	223	ASP	5.0
1	A	98	GLY	4.7
1	A	131	SER	4.4
1	A	95	LEU	4.4
1	A	53	SER	4.3
2	B	97	THR	4.0
1	A	55	ARG	3.8
2	B	217	ASN	3.6
1	A	99	THR	3.6
1	A	54	GLN	3.5
1	A	205	GLU	3.2
2	B	96	ASN	3.0
2	B	225	ALA	2.8
1	A	97	ASP	2.6
1	A	185	PHE	2.5
2	B	220	TRP	2.4
1	A	182	LYS	2.4
1	A	193[A]	ASN	2.4
2	B	94	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	240	ALA	2.3
1	A	134	LYS	2.2
1	A	135	SER	2.2
1	A	67	ASP	2.2
1	A	152	LYS	2.1
1	A	26	THR	2.1
1	A	204	PRO	2.1
1	A	52	SER	2.1
1	A	115	TYR	2.1
2	B	39	MET	2.0
1	A	31	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	SO4	B	245	5/5	0.74	0.35	31,35,40,42	5
3	SO4	B	243	5/5	0.80	0.37	12,15,29,29	5
5	PGE	A	305	10/10	0.80	0.46	19,42,52,53	0
5	PGE	B	302	10/10	0.80	0.23	2,23,30,32	0
4	PG4	A	303	13/13	0.81	0.30	31,38,41,44	0
3	SO4	A	207	5/5	0.84	0.31	18,20,26,26	5
5	PGE	B	301	10/10	0.84	0.24	6,19,28,30	0
5	PGE	A	304	10/10	0.84	0.22	25,44,48,50	0
3	SO4	B	242	5/5	0.85	0.44	20,23,29,32	5
3	SO4	A	206	5/5	0.88	0.43	10,19,25,31	5
3	SO4	B	244	5/5	0.88	0.27	63,65,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.