



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2022 – 02:03 PM EDT

PDB ID : 7RYM  
Title : CD1a-endo-gdTCR complex  
Authors : Wegrecki, M.; Le Nours, J.; Rossjohn, J.  
Deposited on : 2021-08-25  
Resolution : 3.20 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](mailto: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.

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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 : 2.28.1  
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) : 2.28.1

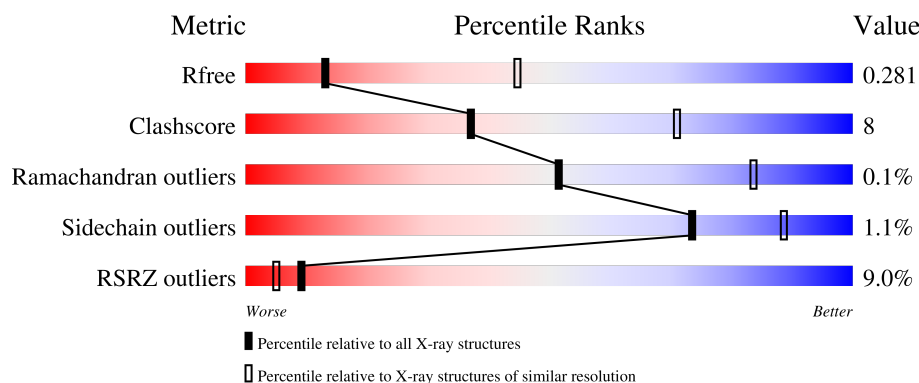
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	286	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>6%</div> </div> </div>
2	B	108	<div> <div>69%</div> <div>21%</div> <div>8%</div> </div>
3	C	248	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
4	D	209	<div> <div>15%</div> <div> <div></div> <div>50%</div> <div>11%</div> <div>38%</div> </div> </div>

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
6	SO4	A	302	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5542 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 surface glycoprotein CD1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2121	1359	368	386	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP P06126
A	0	ALA	-	expression tag	UNP P06126
A	2	THR	ASP	conflict	UNP P06126
A	13	ILE	THR	variant	UNP P06126
A	51	TRP	CYS	variant	UNP P06126
A	279	GLY	-	expression tag	UNP P06126
A	280	SER	-	expression tag	UNP P06126
A	281	LEU	-	expression tag	UNP P06126
A	282	VAL	-	expression tag	UNP P06126
A	283	PRO	-	expression tag	UNP P06126
A	284	ARG	-	expression tag	UNP P06126

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			785	503	135	145	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	-	expression tag	UNP P61769
B	0	ALA	-	expression tag	UNP P61769
B	1	GLY	-	expression tag	UNP P61769
B	101	GLY	-	expression tag	UNP P61769
B	102	SER	-	expression tag	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	103	LEU	-	expression tag	UNP P61769
B	104	VAL	-	expression tag	UNP P61769
B	105	PRO	-	expression tag	UNP P61769
B	106	ARG	-	expression tag	UNP P61769

- Molecule 3 is a protein called T cell receptor gamma variable 4,T cell receptor beta constant 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	235	Total	C	N	O	S	0	0	0
			1712	1091	287	328	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A0C4DH28
C	2	ALA	-	expression tag	UNP A0A0C4DH28
C	103	ASP	-	linker	UNP A0A0C4DH28
C	104	TYR	-	linker	UNP A0A0C4DH28
C	105	TYR	-	linker	UNP A0A0C4DH28
C	106	LYS	-	linker	UNP A0A0C4DH28
C	107	LYS	-	linker	UNP A0A0C4DH28
C	108	LEU	-	linker	UNP A0A0C4DH28
C	109	PHE	-	linker	UNP A0A0C4DH28
C	110	GLY	-	linker	UNP A0A0C4DH28
C	111	SER	-	linker	UNP A0A0C4DH28
C	112	GLY	-	linker	UNP A0A0C4DH28
C	113	THR	-	linker	UNP A0A0C4DH28
C	114	THR	-	linker	UNP A0A0C4DH28
C	115	LEU	-	linker	UNP A0A0C4DH28
C	116	VAL	-	linker	UNP A0A0C4DH28
C	117	VAL	-	linker	UNP A0A0C4DH28
C	118	THR	-	linker	UNP A0A0C4DH28
C	119	GLU	-	linker	UNP A0A0C4DH28
C	122	LYS	ASN	conflict	UNP P01850
C	123	ASN	LYS	conflict	UNP P01850
C	155	TYR	PHE	conflict	UNP P01850
C	175	CYS	SER	engineered mutation	UNP P01850
C	193	ALA	CYS	engineered mutation	UNP P01850

- Molecule 4 is a protein called T cell receptor delta variable 1,T cell receptor alpha chain constant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			912	584	153	171	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A1B0GX56
D	97	LEU	-	linker	UNP A0A1B0GX56
D	98	ARG	-	linker	UNP A0A1B0GX56
D	99	TRP	-	linker	UNP A0A1B0GX56
D	100	PRO	-	linker	UNP A0A1B0GX56
D	101	ASP	-	linker	UNP A0A1B0GX56
D	102	LYS	-	linker	UNP A0A1B0GX56
D	103	LEU	-	linker	UNP A0A1B0GX56
D	104	ILE	-	linker	UNP A0A1B0GX56
D	105	PHE	-	linker	UNP A0A1B0GX56
D	106	GLY	-	linker	UNP A0A1B0GX56
D	107	LYS	-	linker	UNP A0A1B0GX56
D	108	GLY	-	linker	UNP A0A1B0GX56
D	109	THR	-	linker	UNP A0A1B0GX56
D	110	ARG	-	linker	UNP A0A1B0GX56
D	111	VAL	-	linker	UNP A0A1B0GX56
D	112	THR	-	linker	UNP A0A1B0GX56
D	113	VAL	-	linker	UNP A0A1B0GX56
D	114	GLU	-	linker	UNP A0A1B0GX56
D	115	PRO	-	linker	UNP A0A1B0GX56
D	116	ASN	-	linker	UNP A0A1B0GX56
D	163	CYS	THR	engineered mutation	UNP P01848

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

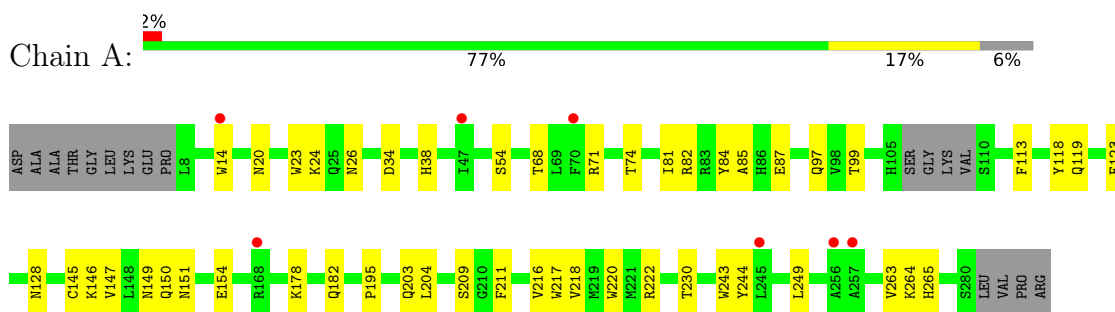


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

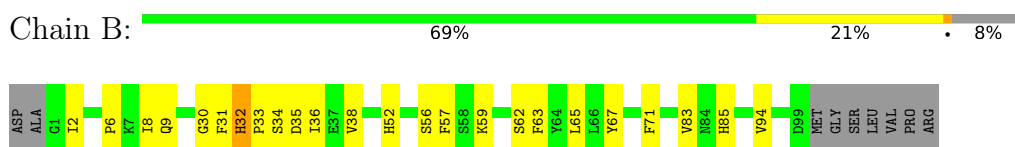
### 3 Residue-property plots [i](#)

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.

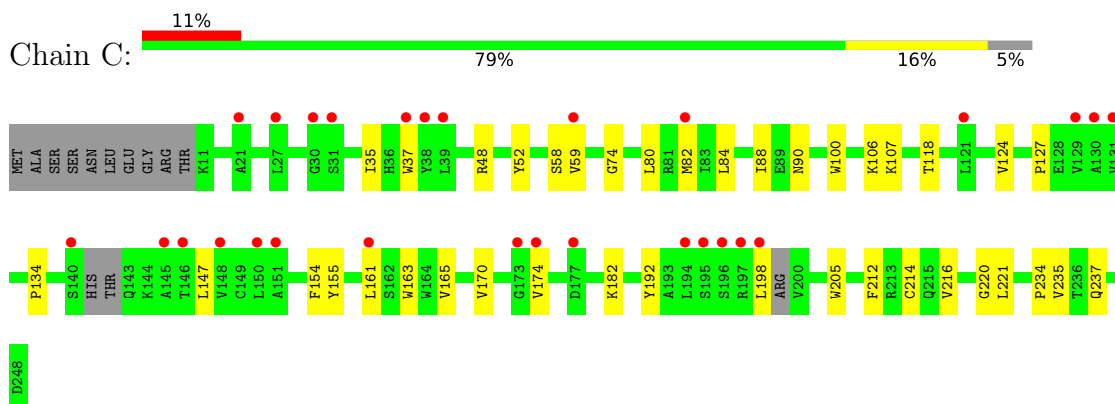
- Molecule 1: T-cell surface glycoprotein CD1a



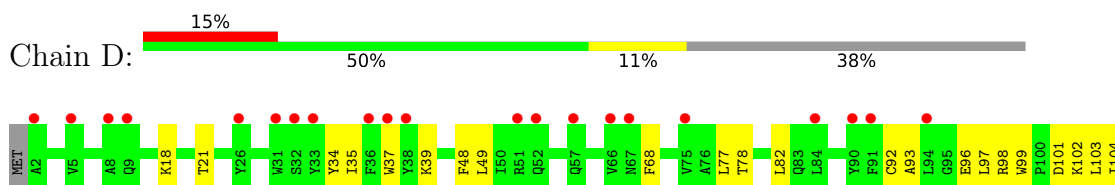
- Molecule 2: Beta-2-microglobulin



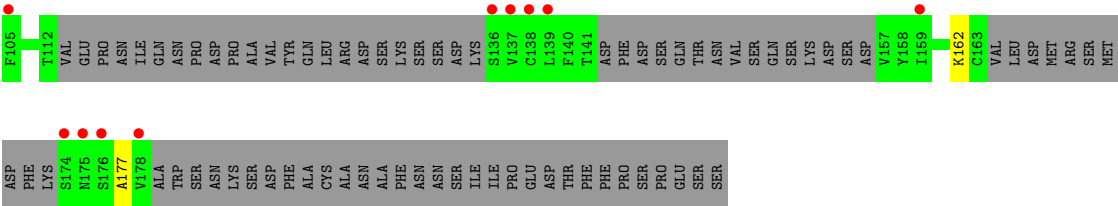
- Molecule 3: T cell receptor gamma variable 4,T cell receptor beta constant 1



- Molecule 4: T cell receptor delta variable 1,T cell receptor alpha chain constant







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	237.08Å 42.46Å 121.59Å 90.00° 116.13° 90.00°	Depositor
Resolution (Å)	41.64 – 3.20 41.64 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.64-3.20) 99.9 (41.64-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.247 , 0.286 0.245 , 0.281	Depositor DCC
$R_{free}$ test set	1029 reflections (5.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.8	Xtriage
Anisotropy	0.996	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4

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	0.24	0/2190	0.49	0/2989
2	B	0.26	0/808	0.51	0/1101
3	C	0.24	0/1755	0.49	0/2408
4	D	0.24	0/929	0.53	0/1267
All	All	0.24	0/5682	0.50	0/7765

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	HIS	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	2121	0	1949	30	0
2	B	785	0	725	20	0
3	C	1712	0	1556	25	0
4	D	912	0	789	17	0
5	A	7	0	10	0	0
6	A	5	0	0	1	0
All	All	5542	0	5029	82	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 (82) 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:20:ASN:ND2	4:D:96:GLU:OE2	2.21	0.73
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.74	0.70
3:C:161:LEU:HG	3:C:216:VAL:HG22	1.73	0.69
3:C:48:ARG:HE	4:D:102:LYS:HB3	1.57	0.67
1:A:195:PRO:O	1:A:203:GLN:NE2	2.28	0.67
1:A:97:GLN:OE1	2:B:32:HIS:NE2	2.24	0.66
4:D:18:LYS:H	4:D:82:LEU:HB3	1.64	0.62
2:B:65:LEU:HD13	2:B:67:TYR:HE1	1.66	0.61
2:B:35:ASP:OD1	4:D:98:ARG:NH2	2.34	0.60
2:B:34:SER:HB2	2:B:63:PHE:CE2	2.37	0.60
1:A:82:ARG:NH2	3:C:58:SER:OG	2.34	0.59
3:C:124:VAL:HG11	3:C:221:LEU:HD11	1.82	0.59
4:D:102:LYS:HE3	4:D:104:ILE:HD11	1.85	0.57
1:A:81:ILE:H	1:A:81:ILE:HD12	1.70	0.56
1:A:82:ARG:HA	1:A:85:ALA:HB2	1.88	0.56
1:A:99:THR:HG22	1:A:113:PHE:HE2	1.71	0.54
1:A:204:LEU:HB3	1:A:220:TRP:CH2	2.44	0.53
6:A:302:SO4:O3	2:B:9:GLN:NE2	2.40	0.53
3:C:37:TRP:CZ2	3:C:82:MET:HB2	2.44	0.53
2:B:8:ILE:HB	2:B:94:VAL:HG21	1.90	0.53
2:B:30:GLY:HA2	2:B:62:SER:OG	2.09	0.52
3:C:170:VAL:HG21	3:C:198:LEU:HD11	1.93	0.51
2:B:56:SER:OG	2:B:57:PHE:N	2.44	0.51
1:A:209:SER:HB3	1:A:244:TYR:HD1	1.74	0.51
2:B:34:SER:O	2:B:34:SER:OG	2.20	0.51
3:C:124:VAL:HG13	3:C:234:PRO:HG2	1.92	0.51
1:A:220:TRP:HD1	1:A:230:THR:HG23	1.77	0.50
1:A:218:VAL:HG22	1:A:263:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:ILE:HD12	4:D:35:ILE:O	2.11	0.50
1:A:81:ILE:O	1:A:82:ARG:HG2	2.12	0.50
2:B:34:SER:HB2	2:B:63:PHE:CD2	2.46	0.50
1:A:119:GLN:O	2:B:2:ILE:HG12	2.13	0.49
3:C:74:GLY:HA3	3:C:80:LEU:HA	1.94	0.49
1:A:71:ARG:HA	1:A:74:THR:HG22	1.94	0.48
4:D:34:TYR:CE1	4:D:97:LEU:HG	2.47	0.48
3:C:88:ILE:HG13	3:C:90:ASN:H	1.78	0.48
4:D:21:THR:HG22	4:D:78:THR:HA	1.95	0.48
3:C:118:THR:HG21	3:C:155:TYR:HE2	1.78	0.48
2:B:38:VAL:HG11	2:B:67:TYR:CE1	2.49	0.48
1:A:147:VAL:HA	1:A:150:GLN:HG2	1.95	0.48
1:A:211:PHE:CE2	1:A:243:TRP:HB2	2.48	0.47
1:A:24:LYS:HZ3	1:A:82:ARG:HD3	1.80	0.47
3:C:182:LYS:HA	3:C:192:TYR:HA	1.97	0.47
2:B:57:PHE:HB3	2:B:63:PHE:CD1	2.51	0.46
1:A:145:CYS:O	1:A:149:ASN:ND2	2.49	0.46
3:C:84:LEU:H	3:C:84:LEU:HD23	1.81	0.46
3:C:163:TRP:HB2	3:C:170:VAL:HG11	1.97	0.46
1:A:38:HIS:NE2	1:A:54:SER:O	2.41	0.45
2:B:36:ILE:HD11	2:B:83:VAL:HG13	1.96	0.45
1:A:146:LYS:HA	1:A:146:LYS:HE3	1.98	0.45
3:C:147:LEU:HD23	3:C:147:LEU:H	1.81	0.45
1:A:178:LYS:O	1:A:182:GLN:HG2	2.16	0.45
1:A:216:VAL:HG12	1:A:265:HIS:CD2	2.52	0.45
3:C:174:VAL:HB	3:C:198:LEU:HG	1.99	0.45
2:B:33:PRO:HG2	2:B:85:HIS:CE1	2.52	0.44
3:C:52:TYR:HD1	3:C:59:VAL:HG22	1.82	0.44
4:D:39:LYS:HB2	4:D:49:LEU:HD21	2.00	0.44
4:D:93:ALA:HB1	4:D:103:LEU:HD23	2.00	0.44
3:C:165:VAL:HG12	3:C:212:PHE:HA	2.00	0.43
1:A:97:GLN:CD	2:B:32:HIS:HE2	2.17	0.43
1:A:84:TYR:HA	1:A:87:GLU:HB2	2.01	0.43
1:A:151:ASN:OD1	1:A:154:GLU:HG2	2.19	0.43
2:B:59:LYS:HE2	2:B:59:LYS:HB3	1.87	0.43
3:C:134:PRO:HG2	3:C:205:TRP:CZ3	2.54	0.43
4:D:37:TRP:CD1	4:D:77:LEU:HB2	2.55	0.42
4:D:162:LYS:HA	4:D:177:ALA:HB2	2.02	0.42
2:B:6:PRO:HB3	2:B:31:PHE:CD1	2.54	0.42
1:A:23:TRP:CG	4:D:99:TRP:HB3	2.55	0.42
3:C:48:ARG:HE	4:D:102:LYS:CB	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:HE1	1:A:26:ASN:HB2	1.85	0.41
2:B:57:PHE:HB3	2:B:63:PHE:CE1	2.54	0.41
3:C:220:GLY:HA3	3:C:234:PRO:O	2.20	0.41
1:A:68:THR:HA	1:A:71:ARG:HG2	2.02	0.41
3:C:35:ILE:HG13	3:C:52:TYR:HB3	2.02	0.41
3:C:127:PRO:HA	3:C:154:PHE:HB3	2.02	0.41
3:C:100:TRP:HA	3:C:107:LYS:HA	2.02	0.41
3:C:106:LYS:HD3	4:D:48:PHE:CD2	2.55	0.41
3:C:235:VAL:O	3:C:237:GLN:HG3	2.21	0.41
1:A:118:TYR:HB3	1:A:123:PHE:CD1	2.56	0.40
4:D:37:TRP:CH2	4:D:92:CYS:HB2	2.56	0.40
2:B:52:HIS:HB3	2:B:67:TYR:CE2	2.56	0.40
4:D:101:ASP:OD1	4:D:102:LYS:N	2.47	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	265/286 (93%)	257 (97%)	7 (3%)	1 (0%)	34	69
2	B	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
3	C	229/248 (92%)	208 (91%)	21 (9%)	0	100	100
4	D	121/209 (58%)	111 (92%)	10 (8%)	0	100	100
All	All	712/851 (84%)	666 (94%)	45 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	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	219/247 (89%)	216 (99%)	3 (1%)	67	86
2	B	83/100 (83%)	82 (99%)	1 (1%)	71	88
3	C	169/215 (79%)	168 (99%)	1 (1%)	86	94
4	D	79/188 (42%)	78 (99%)	1 (1%)	69	87
All	All	550/750 (73%)	544 (99%)	6 (1%)	73	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	222	ARG
1	A	249	LEU
2	B	71	PHE
3	C	214	CYS
4	D	68	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

2 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	$\# Z  > 2$
6	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
5	PEG	A	301	-	6,6,6	0.10	0	5,5,5	0.09	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
5	PEG	A	301	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	SO4	1	0

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	269/286 (94%)	0.10	7 (2%) 56 40	61, 98, 137, 167	0
2	B	99/108 (91%)	-0.03	0 100 100	62, 88, 125, 129	0
3	C	235/248 (94%)	0.55	28 (11%) 4 2	93, 164, 217, 226	0
4	D	129/209 (61%)	0.69	31 (24%) 0 0	106, 175, 210, 224	0
All	All	732/851 (86%)	0.33	66 (9%) 9 5	61, 125, 207, 226	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	195	SER	10.3
3	C	194	LEU	8.0
3	C	131	VAL	5.1
4	D	32	SER	5.0
4	D	159	ILE	4.7
3	C	174	VAL	4.3
4	D	5	VAL	4.3
3	C	146	THR	4.0
4	D	139	LEU	3.9
3	C	196	SER	3.6
4	D	105	PHE	3.5
3	C	140	SER	3.5
3	C	38	TYR	3.5
4	D	8	ALA	3.4
3	C	27	LEU	3.4
4	D	91	PHE	3.2
3	C	21	ALA	3.1
3	C	148	VAL	3.1
4	D	175	ASN	3.1
3	C	198	LEU	3.0
4	D	33	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	178	VAL	3.0
3	C	151	ALA	3.0
4	D	38	TYR	2.8
3	C	150	LEU	2.8
4	D	174	SER	2.8
3	C	59	VAL	2.8
4	D	94	LEU	2.7
3	C	30	GLY	2.7
3	C	37	TRP	2.7
3	C	39	LEU	2.7
4	D	84	LEU	2.7
4	D	67	ASN	2.7
3	C	130	ALA	2.7
4	D	138	CYS	2.6
3	C	173	GLY	2.6
3	C	145	ALA	2.6
1	A	70	PHE	2.6
4	D	57	GLN	2.5
1	A	47	ILE	2.5
3	C	82	MET	2.5
4	D	2	ALA	2.5
4	D	136	SER	2.5
4	D	66	VAL	2.4
4	D	51	ARG	2.4
3	C	177	ASP	2.4
1	A	168	ARG	2.4
4	D	90	TYR	2.3
4	D	36	PHE	2.3
4	D	137	VAL	2.3
3	C	161	LEU	2.3
1	A	257	ALA	2.3
3	C	129	VAL	2.2
4	D	52	GLN	2.2
4	D	26	TYR	2.2
3	C	31	SER	2.2
4	D	75	VAL	2.2
4	D	37	TRP	2.1
4	D	9	GLN	2.1
1	A	14	TRP	2.1
1	A	256	ALA	2.1
4	D	176	SER	2.1
3	C	197	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	31	TRP	2.0
1	A	245	LEU	2.0
3	C	121	LEU	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	302	5/5	0.69	0.50	86,88,121,174	0
5	PEG	A	301	7/7	0.89	0.29	69,86,88,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.