



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 02:03 PM EST

PDB ID : 6UJ8
Title : Crystal structure of HLA-B*07:02 with wild-type IDH2 peptide
Authors : Miller, M.S.; Thirawatananond, P.; Gabelli, S.B.
Deposited on : 2019-10-02
Resolution : 2.25 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 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 : 2.23.2
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) : 2.23.2

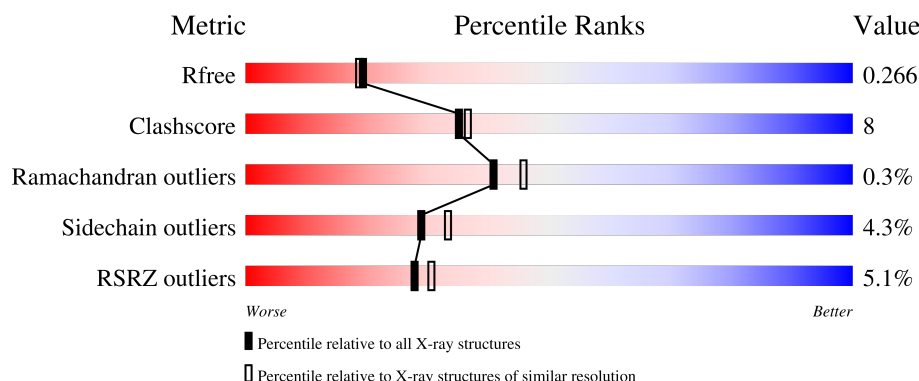
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	298	<div> <div>2%</div> <div>76%</div> <div>15%</div> <div>8%</div> </div>
1	D	298	<div> <div>9%</div> <div>73%</div> <div>18%</div> <div>8%</div> </div>
2	B	119	<div> <div>2%</div> <div>69%</div> <div>16%</div> <div>15%</div> </div>
2	E	119	<div> <div>3%</div> <div>72%</div> <div>12%</div> <div>15%</div> </div>
3	C	10	<div> <div>70%</div> <div>30%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	10	 <div>90%10%</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
4	PEG	B	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6620 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 HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2258	1402	413	437	6			
1	D	275	Total	C	N	O	S	0	0	0
			2258	1402	413	437	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01889
A	281	GLY	-	expression tag	UNP P01889
A	282	SER	-	expression tag	UNP P01889
A	283	LEU	-	expression tag	UNP P01889
A	284	HIS	-	expression tag	UNP P01889
A	285	HIS	-	expression tag	UNP P01889
A	286	ILE	-	expression tag	UNP P01889
A	287	LEU	-	expression tag	UNP P01889
A	288	ASP	-	expression tag	UNP P01889
A	289	ALA	-	expression tag	UNP P01889
A	290	GLN	-	expression tag	UNP P01889
A	291	LYS	-	expression tag	UNP P01889
A	292	MET	-	expression tag	UNP P01889
A	293	VAL	-	expression tag	UNP P01889
A	294	TRP	-	expression tag	UNP P01889
A	295	ASN	-	expression tag	UNP P01889
A	296	HIS	-	expression tag	UNP P01889
A	297	ARG	-	expression tag	UNP P01889
D	0	MET	-	initiating methionine	UNP P01889
D	281	GLY	-	expression tag	UNP P01889
D	282	SER	-	expression tag	UNP P01889
D	283	LEU	-	expression tag	UNP P01889
D	284	HIS	-	expression tag	UNP P01889
D	285	HIS	-	expression tag	UNP P01889
D	286	ILE	-	expression tag	UNP P01889

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Chain	Residue	Modelled	Actual	Comment	Reference
D	287	LEU	-	expression tag	UNP P01889
D	288	ASP	-	expression tag	UNP P01889
D	289	ALA	-	expression tag	UNP P01889
D	290	GLN	-	expression tag	UNP P01889
D	291	LYS	-	expression tag	UNP P01889
D	292	MET	-	expression tag	UNP P01889
D	293	VAL	-	expression tag	UNP P01889
D	294	TRP	-	expression tag	UNP P01889
D	295	ASN	-	expression tag	UNP P01889
D	296	HIS	-	expression tag	UNP P01889
D	297	ARG	-	expression tag	UNP P01889

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			843	536	142	162	3			
2	E	101	Total	C	N	O	S	0	0	0
			843	536	142	162	3			

- Molecule 3 is a protein called Isocitrate dehydrogenase [NADP], mitochondrial.

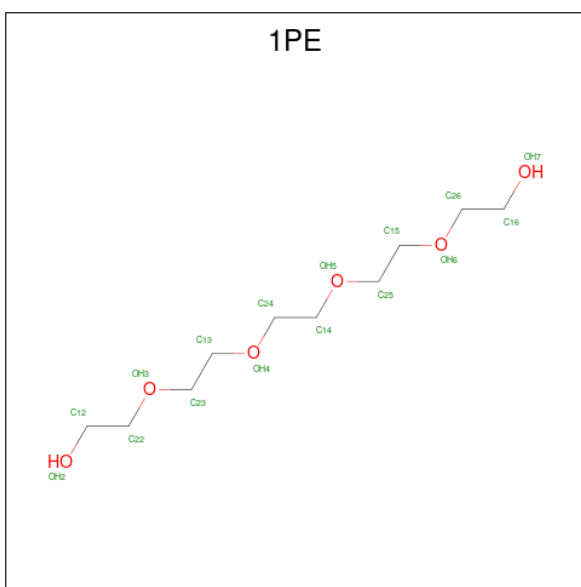
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			76	46	15	15			
3	F	10	Total	C	N	O	0	0	0
			76	46	15	15			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



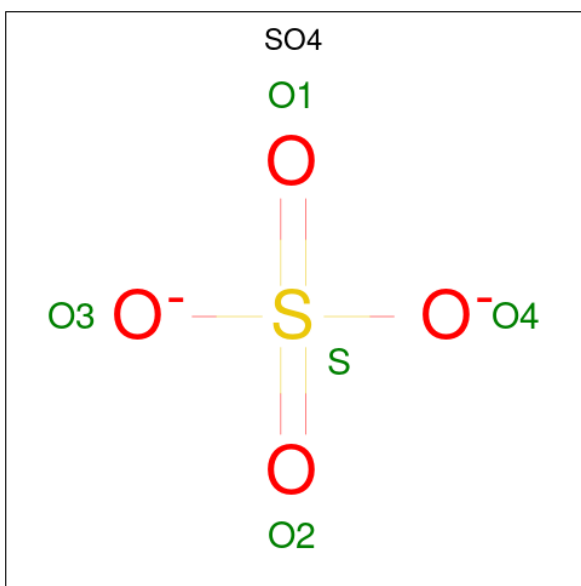
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



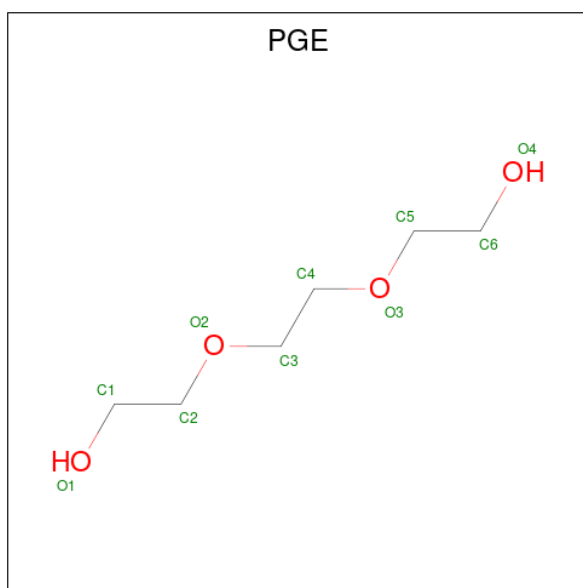
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



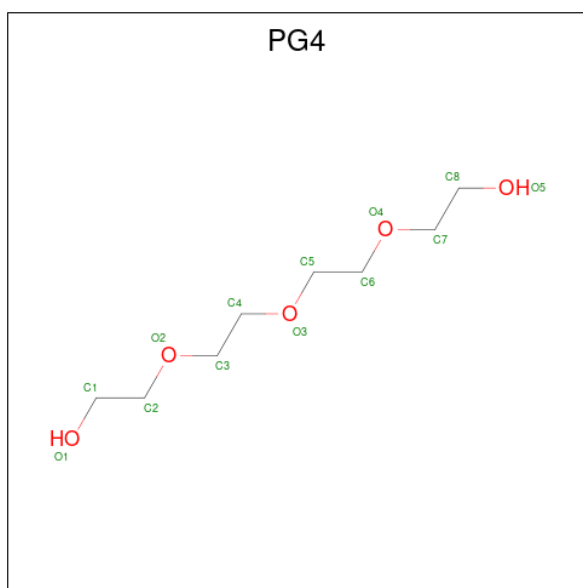
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

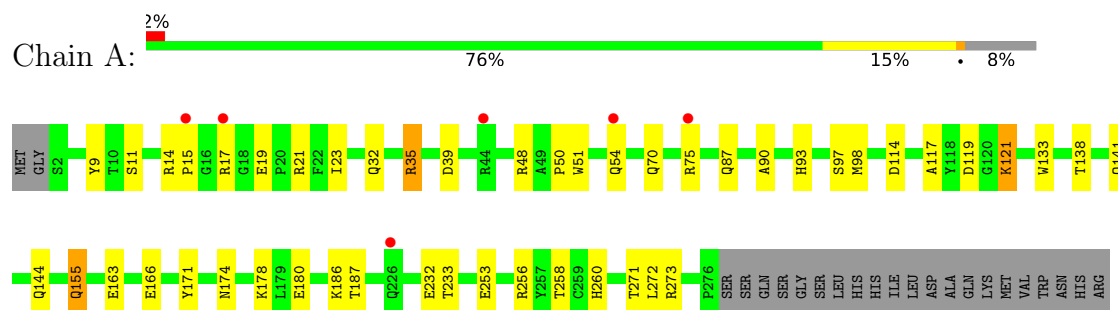
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	59	Total 59	O 59	0	0
9	B	20	Total 20	O 20	0	0
9	C	1	Total 1	O 1	0	0
9	D	52	Total 52	O 52	0	0
9	E	34	Total 34	O 34	0	0
9	F	4	Total 4	O 4	0	0

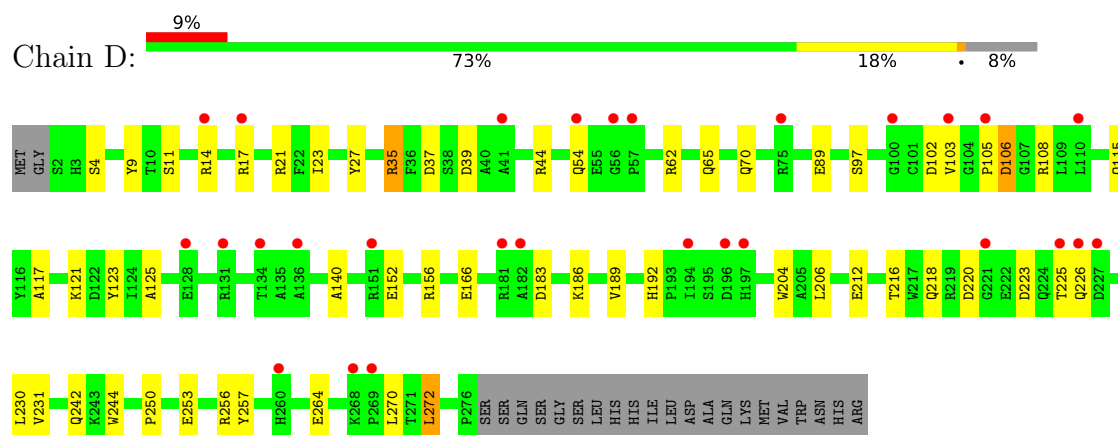
3 Residue-property plots [i](#)

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.

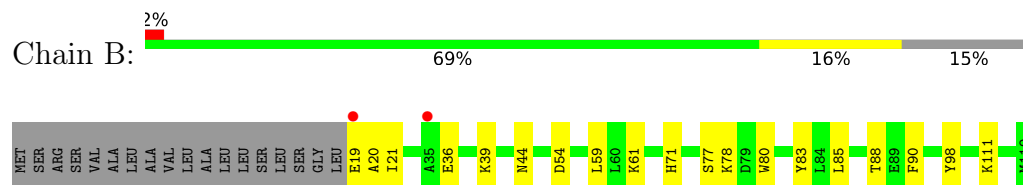
- Molecule 1: HLA class I histocompatibility antigen, B-7 alpha chain



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- Molecule 2: Beta-2-microglobulin

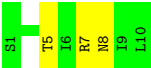


- Molecule 2: Beta-2-microglobulin

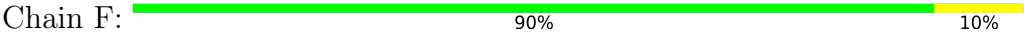




● Molecule 3: Isocitrate dehydrogenase [NADP], mitochondrial



● Molecule 3: Isocitrate dehydrogenase [NADP], mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.69Å 70.48Å 88.15Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	47.58 – 2.25 47.58 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.58-2.25) 99.8 (47.58-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.216 , 0.260 0.223 , 0.266	Depositor DCC
R_{free} test set	1884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6620	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, PGE, 1PE, PEG, 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	0.67	0/2321	0.84	0/3154
1	D	0.64	0/2321	0.87	0/3154
2	B	0.64	0/866	0.83	0/1171
2	E	0.64	0/866	0.82	0/1171
3	C	0.69	0/76	0.96	0/101
3	F	0.76	0/76	0.86	0/101
All	All	0.65	0/6526	0.85	0/8852

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 [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	2258	0	2099	40	0
1	D	2258	0	2099	37	0
2	B	843	0	802	20	0
2	E	843	0	802	13	0
3	C	76	0	82	4	0
3	F	76	0	82	0	0
4	A	14	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	20	7	0
4	D	7	0	10	3	0
4	E	7	0	10	0	0
5	A	16	0	22	3	0
6	A	10	0	0	1	0
6	D	5	0	0	0	0
7	B	10	0	14	0	0
8	D	13	0	18	5	0
9	A	59	0	0	2	0
9	B	20	0	0	0	0
9	C	1	0	0	0	0
9	D	52	0	0	5	0
9	E	34	0	0	1	0
9	F	4	0	0	0	0
All	All	6620	0	6080	103	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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLU:HG2	2:B:20:ALA:H	1.15	1.07
2:E:19:GLU:N	2:E:19:GLU:OE1	2.10	0.85
1:A:187:THR:HB	1:A:272:LEU:HD11	1.60	0.84
2:B:19:GLU:HG2	2:B:20:ALA:N	1.95	0.81
1:A:15:PRO:HB3	1:A:90:ALA:O	1.80	0.80
2:B:77:SER:HB3	4:B:201:PEG:H31	1.65	0.77
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.66	0.77
2:B:19:GLU:CG	2:B:20:ALA:H	1.94	0.76
1:A:119:ASP:HB3	2:B:20:ALA:HB3	1.69	0.74
2:B:111:LYS:HD2	4:B:203:PEG:H42	1.70	0.73
1:A:155:GLN:HG3	3:C:5:THR:HG21	1.69	0.72
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.73	0.72
1:D:21:ARG:NH1	1:D:39:ASP:OD2	2.23	0.71
1:D:21:ARG:HE	1:D:23:ILE:HD11	1.57	0.69
5:A:302:1PE:H152	2:B:83:TYR:CE1	2.28	0.67
1:A:35:ARG:HG2	1:A:48:ARG:HD3	1.77	0.67
1:D:121:LYS:HG3	2:E:21:ILE:HG13	1.78	0.66
1:D:212:GLU:HG2	9:D:432:HOH:O	1.96	0.64
2:B:111:LYS:CD	4:B:203:PEG:H42	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLN:HG3	9:D:444:HOH:O	1.97	0.64
2:B:78:LYS:HG3	4:B:201:PEG:H22	1.80	0.62
1:A:54:GLN:OE1	1:A:174:ASN:HB3	2.01	0.61
4:D:302:PEG:H42	9:D:447:HOH:O	1.99	0.60
1:A:260:HIS:NE2	1:A:271:THR:OG1	2.32	0.60
8:D:301:PG4:H82	4:D:302:PEG:O1	2.03	0.59
8:D:301:PG4:H82	8:D:301:PG4:C5	2.34	0.58
2:E:21:ILE:HG22	2:E:21:ILE:O	2.02	0.58
1:A:114:ASP:OD1	3:C:7:ARG:NH2	2.36	0.58
1:D:14:ARG:HB3	1:D:17:ARG:HB2	1.86	0.58
2:B:71:HIS:HA	2:B:85:LEU:O	2.03	0.58
1:D:166:GLU:HG2	9:D:450:HOH:O	2.03	0.58
1:D:231:VAL:HG11	1:D:244:TRP:CE2	2.38	0.57
2:B:77:SER:HB3	4:B:201:PEG:C3	2.33	0.55
1:A:9:TYR:CE2	1:A:70:GLN:HG2	2.42	0.55
2:B:36:GLU:OE1	2:B:39:LYS:HD2	2.07	0.55
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.23	0.54
1:D:218:GLN:O	1:D:257:TYR:HA	2.07	0.53
1:A:260:HIS:CD2	1:A:271:THR:OG1	2.61	0.53
1:D:35:ARG:HD2	1:D:35:ARG:C	2.29	0.53
1:D:35:ARG:HG3	2:E:73:ASP:CG	2.29	0.53
1:D:231:VAL:HG11	1:D:244:TRP:CZ2	2.44	0.53
1:A:260:HIS:CD2	1:A:271:THR:HG1	2.25	0.53
1:A:233:THR:N	6:A:304:SO4:O1	2.24	0.52
2:E:105:VAL:HG23	9:E:304:HOH:O	2.08	0.52
1:D:152:GLU:OE1	1:D:156:ARG:NH2	2.36	0.52
1:D:152:GLU:OE1	1:D:156:ARG:NE	2.42	0.52
1:A:14:ARG:NH2	1:A:39:ASP:OD2	2.43	0.51
1:D:220:ASP:OD2	1:D:256:ARG:NH1	2.44	0.51
8:D:301:PG4:H82	8:D:301:PG4:H52	1.94	0.49
1:D:4:SER:HB3	1:D:102:ASP:OD1	2.13	0.49
1:D:27:TYR:CD2	8:D:301:PG4:H32	2.48	0.48
1:D:65:GLN:O	1:D:65:GLN:NE2	2.45	0.48
2:B:59:LEU:HD13	2:B:88:THR:HG22	1.96	0.48
2:E:47:VAL:HG23	2:E:50:PHE:CE1	2.49	0.48
1:D:21:ARG:NH2	1:D:37:ASP:OD2	2.47	0.48
1:A:121:LYS:HG2	2:B:21:ILE:HD12	1.95	0.48
1:A:19:GLU:HB3	1:A:75:ARG:NH1	2.30	0.47
1:A:163:GLU:OE1	4:A:303:PEG:H42	2.15	0.47
1:D:192:HIS:CE1	2:E:118:ASP:HB3	2.50	0.47
1:D:220:ASP:OD2	1:D:256:ARG:NE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HA	1:A:141:GLN:NE2	2.31	0.46
1:D:9:TYR:CE2	1:D:70:GLN:HG2	2.50	0.46
1:D:250:PRO:HB2	1:D:253:GLU:HG3	1.97	0.46
1:D:117:ALA:HB2	2:E:80:TRP:CE2	2.51	0.46
1:D:44:ARG:NH1	9:D:408:HOH:O	2.49	0.46
2:E:71:HIS:HA	2:E:85:LEU:O	2.15	0.46
5:A:302:1PE:H152	2:B:83:TYR:HE1	1.77	0.45
1:D:231:VAL:CG1	1:D:244:TRP:CZ2	3.00	0.45
1:A:48:ARG:HH21	5:A:302:1PE:H122	1.81	0.45
1:A:180:GLU:OE2	9:A:401:HOH:O	2.21	0.45
2:B:44:ASN:HB3	2:B:85:LEU:HD11	1.99	0.45
1:D:189:VAL:HG23	1:D:272:LEU:HD23	1.99	0.45
1:A:70:GLN:OE1	3:C:7:ARG:HD3	2.17	0.45
2:B:61:LYS:HG3	2:B:98:TYR:CE2	2.53	0.44
1:D:105:PRO:HG2	1:D:105:PRO:O	2.18	0.44
1:D:204:TRP:HZ2	2:E:118:ASP:O	2.01	0.43
1:A:54:GLN:OE1	1:A:174:ASN:CB	2.64	0.43
2:E:47:VAL:HG23	2:E:50:PHE:HE1	1.84	0.43
1:A:133:TRP:O	1:A:144:GLN:NE2	2.52	0.43
1:A:186:LYS:HG2	1:D:54:GLN:CG	2.49	0.43
2:E:21:ILE:HD13	2:E:21:ILE:HA	1.96	0.43
2:E:75:SER:HB3	2:E:83:TYR:CE1	2.54	0.43
1:A:51:TRP:CZ3	1:A:171:TYR:HB3	2.54	0.43
1:A:232:GLU:CD	9:A:404:HOH:O	2.57	0.43
1:D:115:GLN:HB3	1:D:125:ALA:HA	2.00	0.43
1:A:117:ALA:HB2	2:B:80:TRP:CD2	2.55	0.42
1:A:50:PRO:O	1:D:186:LYS:HD3	2.19	0.42
8:D:301:PG4:C8	4:D:302:PEG:O1	2.67	0.42
1:A:155:GLN:CG	3:C:5:THR:HG21	2.45	0.42
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.49	0.42
1:D:37:ASP:OD1	1:D:39:ASP:HB2	2.20	0.42
1:A:54:GLN:OE1	1:A:174:ASN:CG	2.58	0.41
1:A:87:GLN:NE2	2:B:19:GLU:OE1	2.54	0.41
1:A:187:THR:CB	1:A:272:LEU:HD11	2.41	0.41
1:A:258:THR:HG22	1:A:273:ARG:HG3	2.01	0.41
2:B:111:LYS:HD3	4:B:203:PEG:O2	2.21	0.41
1:D:206:LEU:HD23	1:D:242:GLN:HG2	2.02	0.41
1:A:166:GLU:HB3	4:A:303:PEG:C2	2.51	0.41
1:A:186:LYS:HG2	1:D:54:GLN:HG3	2.02	0.40
1:A:253:GLU:O	1:A:256:ARG:HB2	2.21	0.40
4:B:201:PEG:H12	4:B:201:PEG:H32	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HE2	1:D:183:ASP:OD2	2.21	0.40
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.56	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	273/298 (92%)	267 (98%)	6 (2%)	0	100	100
1	D	273/298 (92%)	266 (97%)	6 (2%)	1 (0%)	34	37
2	B	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
2	E	99/119 (83%)	98 (99%)	0	1 (1%)	15	13
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	760/854 (89%)	745 (98%)	13 (2%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	ASP
2	E	21	ILE

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	234/254 (92%)	228 (97%)	6 (3%)	46	55
1	D	234/254 (92%)	219 (94%)	15 (6%)	17	16
2	B	95/109 (87%)	93 (98%)	2 (2%)	53	62
2	E	95/109 (87%)	91 (96%)	4 (4%)	30	34
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	4
3	F	9/9 (100%)	8 (89%)	1 (11%)	6	4
All	All	676/744 (91%)	647 (96%)	29 (4%)	29	33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	ARG
1	A	97	SER
1	A	98	MET
1	A	121	LYS
1	A	155	GLN
2	B	54	ASP
2	B	90	PHE
3	C	8	ASN
1	D	11	SER
1	D	35	ARG
1	D	62	ARG
1	D	89	GLU
1	D	97	SER
1	D	103	VAL
1	D	106	ASP
1	D	108	ARG
1	D	216	THR
1	D	223	ASP
1	D	225	THR
1	D	230	LEU
1	D	264	GLU
1	D	270	LEU
1	D	272	LEU
2	E	21	ILE
2	E	40	SER
2	E	69	VAL
2	E	90	PHE
3	F	8	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	144	GLN
1	D	65	GLN
1	D	127	ASN
1	D	141	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
4	PEG	A	301	-	6,6,6	0.27	0	5,5,5	0.13	0
4	PEG	E	201	-	6,6,6	0.24	0	5,5,5	0.15	0
8	PG4	D	301	-	12,12,12	0.21	0	11,11,11	0.19	0
4	PEG	A	303	-	6,6,6	0.15	0	5,5,5	0.16	0
4	PEG	B	201	-	6,6,6	0.36	0	5,5,5	0.13	0
4	PEG	D	302	-	6,6,6	0.27	0	5,5,5	0.17	0
6	SO4	D	303	-	4,4,4	0.35	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	305	-	4,4,4	0.35	0	6,6,6	0.04	0
4	PEG	B	203	-	6,6,6	0.11	0	5,5,5	0.18	0
7	PGE	B	202	-	9,9,9	0.16	0	8,8,8	0.16	0
5	1PE	A	302	-	15,15,15	0.62	0	14,14,14	0.58	0
6	SO4	A	304	-	4,4,4	0.35	0	6,6,6	0.13	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	PEG	A	301	-	-	1/4/4/4	-
4	PEG	E	201	-	-	3/4/4/4	-
8	PG4	D	301	-	-	2/10/10/10	-
4	PEG	A	303	-	-	1/4/4/4	-
4	PEG	B	201	-	-	1/4/4/4	-
4	PEG	D	302	-	-	1/4/4/4	-
4	PEG	B	203	-	-	1/4/4/4	-
7	PGE	B	202	-	-	4/7/7/7	-
5	1PE	A	302	-	-	9/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	302	PEG	C4-C3-O2-C2
5	A	302	1PE	OH4-C13-C23-OH3
8	D	301	PG4	O3-C5-C6-O4
5	A	302	1PE	OH5-C14-C24-OH4
5	A	302	1PE	OH7-C16-C26-OH6
4	B	201	PEG	C1-C2-O2-C3
5	A	302	1PE	OH2-C12-C22-OH3
7	B	202	PGE	O1-C1-C2-O2
4	A	301	PEG	O1-C1-C2-O2
7	B	202	PGE	O3-C5-C6-O4
8	D	301	PG4	O2-C3-C4-O3
4	B	203	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	E	201	PEG	O2-C3-C4-O4
5	A	302	1PE	C12-C22-OH3-C23
5	A	302	1PE	C24-C14-OH5-C25
7	B	202	PGE	C3-C4-O3-C5
5	A	302	1PE	C15-C25-OH5-C14
5	A	302	1PE	C23-C13-OH4-C24
4	E	201	PEG	O1-C1-C2-O2
4	E	201	PEG	C4-C3-O2-C2
5	A	302	1PE	C13-C23-OH3-C22
4	A	303	PEG	C1-C2-O2-C3
7	B	202	PGE	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	301	PG4	5	0
4	A	303	PEG	2	0
4	B	201	PEG	4	0
4	D	302	PEG	3	0
4	B	203	PEG	3	0
5	A	302	1PE	3	0
6	A	304	SO4	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, 95th 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	275/298 (92%)	0.40	6 (2%) 62 65	22, 41, 71, 99	0
1	D	275/298 (92%)	0.56	28 (10%) 6 6	24, 47, 78, 98	0
2	B	101/119 (84%)	0.11	2 (1%) 65 68	23, 34, 56, 75	0
2	E	101/119 (84%)	0.24	3 (2%) 50 53	25, 42, 69, 80	0
3	C	10/10 (100%)	0.22	0 100 100	26, 40, 45, 47	0
3	F	10/10 (100%)	0.12	0 100 100	34, 40, 45, 47	0
All	All	772/854 (90%)	0.39	39 (5%) 28 30	22, 42, 73, 99	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	GLU	5.8
2	E	19	GLU	5.6
1	D	14	ARG	5.4
1	D	194	ILE	4.9
1	A	17	ARG	4.2
1	D	131	ARG	4.2
1	D	136	ALA	4.0
1	D	269	PRO	4.0
1	D	268	LYS	3.9
1	D	260	HIS	3.6
1	D	221	GLY	3.5
1	D	105	PRO	3.3
1	A	15	PRO	3.1
1	D	57	PRO	2.8
1	A	44	ARG	2.8
1	D	100	GLY	2.7
1	D	226	GLN	2.7
1	A	75	ARG	2.6
1	D	75	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLN	2.5
1	D	134	THR	2.5
1	D	103	VAL	2.5
1	D	56	GLY	2.5
1	D	225	THR	2.5
1	D	182	ALA	2.5
1	D	128	GLU	2.4
2	E	20	ALA	2.4
1	D	17	ARG	2.4
1	D	54	GLN	2.4
1	D	181	ARG	2.4
1	D	197	HIS	2.4
1	D	151	ARG	2.3
2	B	35	ALA	2.3
1	D	110	LEU	2.2
1	D	196	ASP	2.2
1	A	226	GLN	2.2
1	D	41	ALA	2.2
2	E	68	LYS	2.1
1	D	227	ASP	2.1

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, 95th 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	PEG	E	201	7/7	0.46	0.30	68,69,79,82	0
6	SO4	A	305	5/5	0.66	0.30	88,96,104,108	0
5	1PE	A	302	16/16	0.78	0.26	48,55,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PEG	B	201	7/7	0.81	0.24	61,63,72,74	0
4	PEG	A	303	7/7	0.82	0.25	68,73,78,79	0
4	PEG	B	203	7/7	0.84	0.18	55,58,65,67	0
8	PG4	D	301	13/13	0.85	0.17	59,63,73,79	0
4	PEG	D	302	7/7	0.89	0.23	60,63,68,68	0
6	SO4	D	303	5/5	0.90	0.14	93,96,106,109	0
6	SO4	A	304	5/5	0.90	0.28	62,69,72,80	0
4	PEG	A	301	7/7	0.91	0.24	44,47,61,65	0
7	PGE	B	202	10/10	0.94	0.17	38,45,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.