Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 07:05 PM EDT

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 (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 (i)) were used in the production of this report:

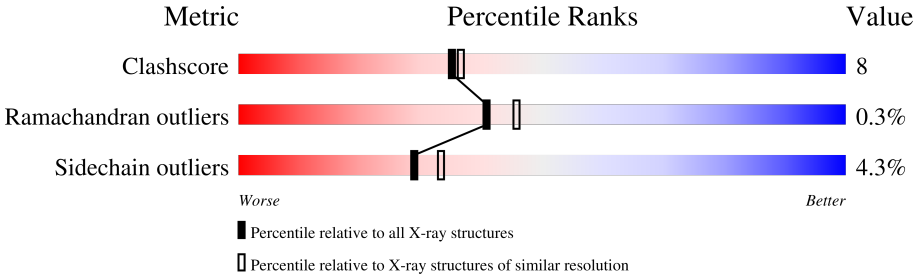
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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

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 (i)

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
			Total	C	N	O	S			
1	A	275	2258	1402	413	437	6	0	0	0
1	D	275	2258	1402	413	437	6	0	0	0

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

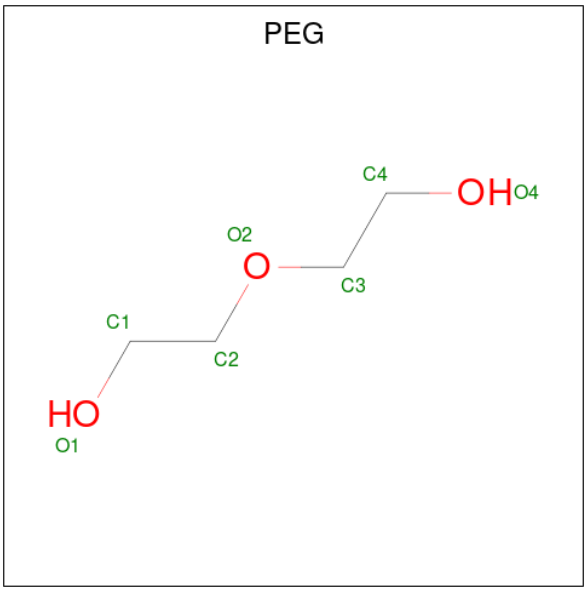
- Molecule 2 is a protein called Beta-2-microglobulin.

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

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

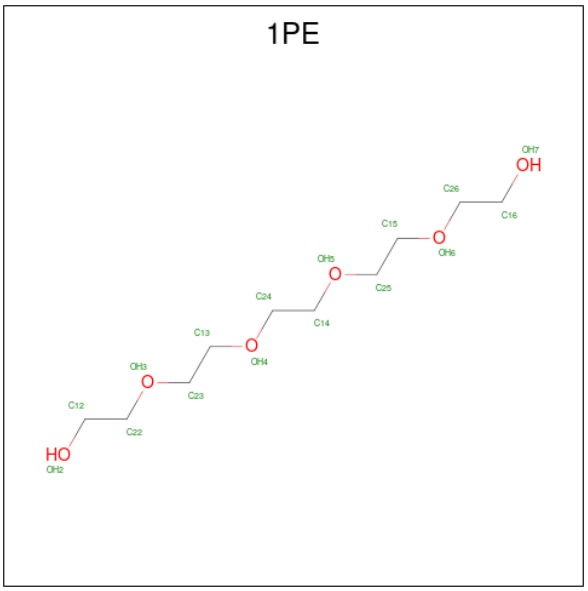
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	76	46	15	15	0	0	0
3	F	10	76	46	15	15	0	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



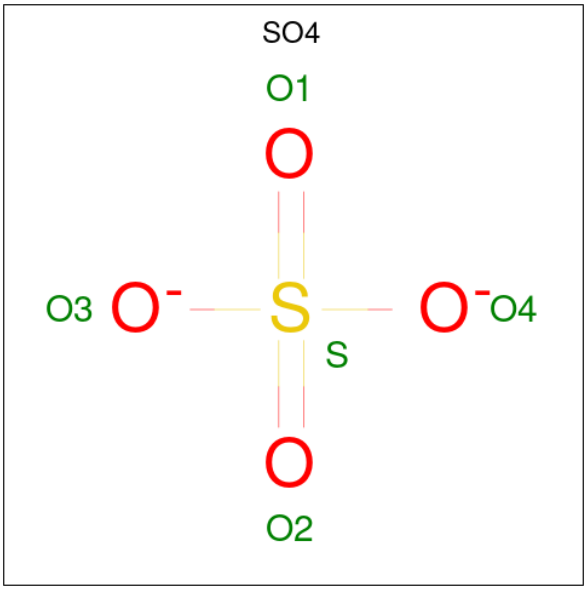
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	A	1	7	4	3	0	0
			Total	C	O		
4	B	1	7	4	3	0	0
			Total	C	O		
4	B	1	7	4	3	0	0
			Total	C	O		
4	D	1	7	4	3	0	0
			Total	C	O		
4	E	1	7	4	3	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



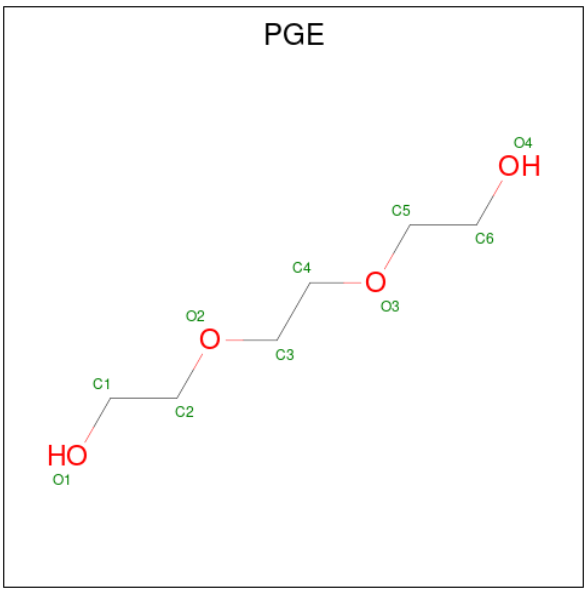
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	16	10	6	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



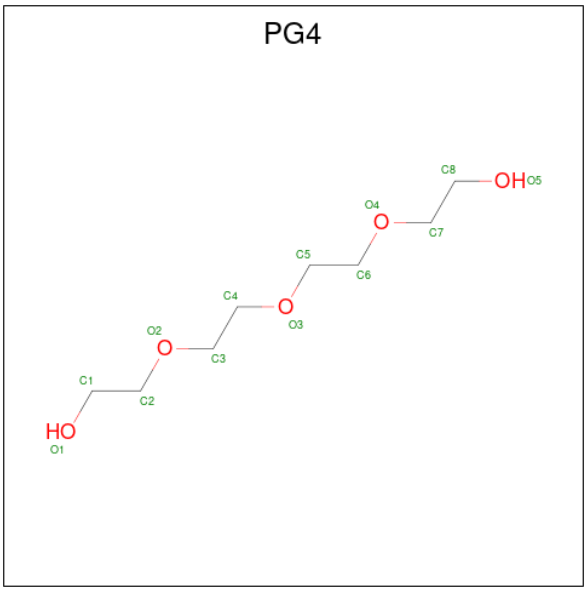
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	A	1	5	4	1	0	0
			Total	O	S		
6	D	1	5	4	1	0	0

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



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

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



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

- Molecule 9 is water.

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

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	99.8 (47.58-2.25)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.216 , 0.260	Depositor
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.133	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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.*

[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.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PGE, PEG, PG4, 1PE

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.

4.2 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.

4.3 Torsion angles (i)

4.3.1 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

4.3.2 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

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

12 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.