Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2024 – 07:12 pm BST

PDB ID	:	8PJG
Title	:	F11 TCR in complex with Human Leukocyte Antigen class II allotype DR1 presenting P11T->R modified influenza A virus haemagglutinin (HA)306-318 PKYVKQNTLKLAR
Authors	:	MacLachlan, B.J.; Wall, A.; Greenshields-Watson, A.L.; Cole, D.K.; Rizkallah, P.J.; Godkin, A.J.
Deposited on	:	2023-06-23
Resolution	:	1.83 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:

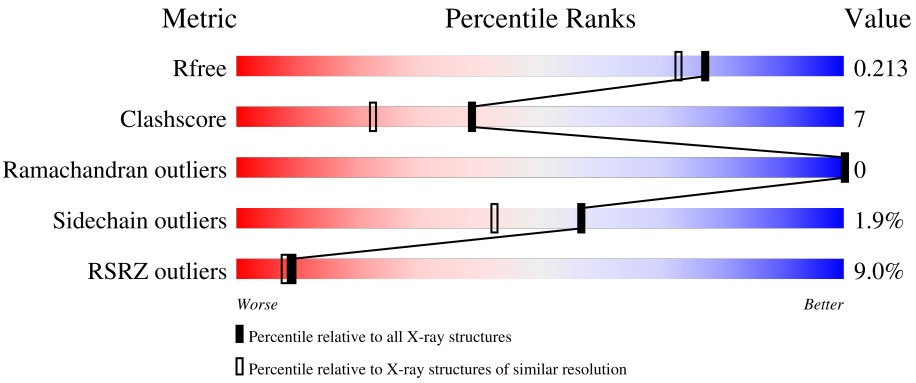
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	183	10% 87% 9%
2	B	191	26% 75% 24%
3	C	13	8% 85% 15%
4	D	207	% 84% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	241	

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	EDO	D	301	-	-	X	-
6	EDO	E	303	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7240 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	1	0
			1561	983	279	293	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01911
B	11	LEU	PRO	variant	UNP P01911
B	13	PHE	ARG	variant	UNP P01911
B	26	LEU	PHE	variant	UNP P01911
B	28	GLU	ASP	variant	UNP P01911
B	30	CYS	TYR	variant	UNP P01911
B	31	ILE	PHE	variant	UNP P01911
B	47	TYR	PHE	variant	UNP P01911
B	67	LEU	ILE	variant	UNP P01911
B	71	ARG	ALA	variant	UNP P01911
B	86	GLY	VAL	variant	UNP P01911
B	96	GLU	GLN	variant	UNP P01911
B	133	ARG	LEU	variant	UNP P01911
B	142	VAL	MET	variant	UNP P01911

- Molecule 3 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			110	71	21	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	13	ARG	THR	engineered mutation	UNP P03435

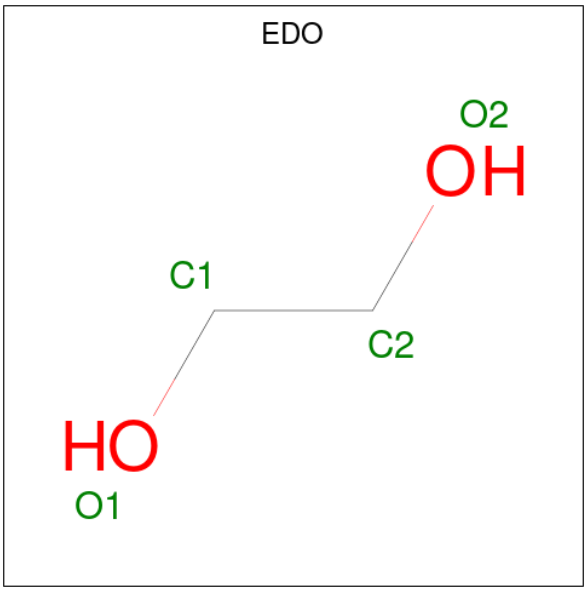
- Molecule 4 is a protein called T cell receptor alpha chain constant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	203	Total	C	N	O	S	0	8	0
			1635	1034	271	321	9			

- Molecule 5 is a protein called T cell receptor beta constant 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	9	0
			1967	1234	346	378	9			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



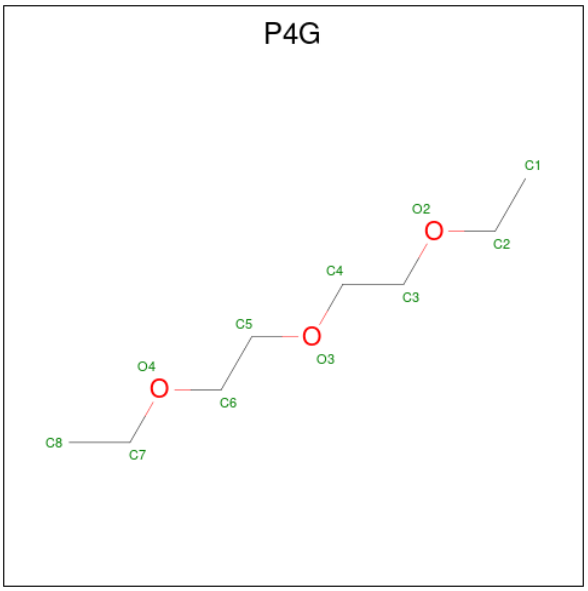
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0
6	E	1	Total 4	C 2	O 2	0	0

- Molecule 7 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 11 8 3	0	0
7	E	1	Total C O 11 8 3	0	0

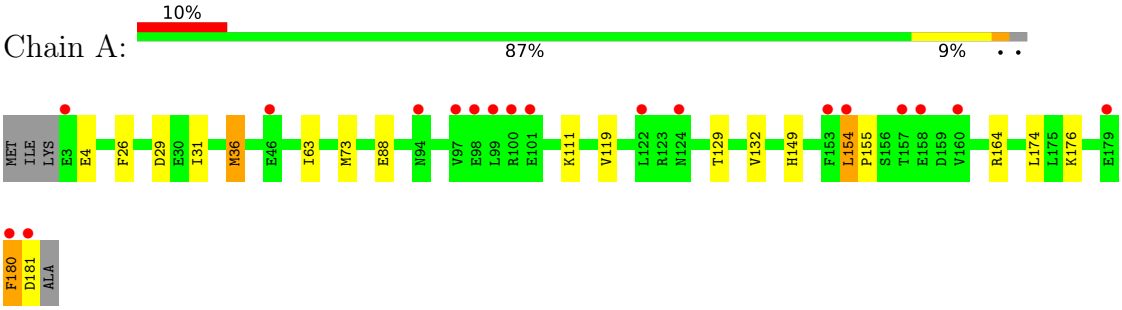
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	38	Total O 38 38	0	0
8	B	32	Total O 32 32	0	0
8	C	9	Total O 9 9	0	0
8	D	148	Total O 148 148	0	0
8	E	185	Total O 185 185	0	0

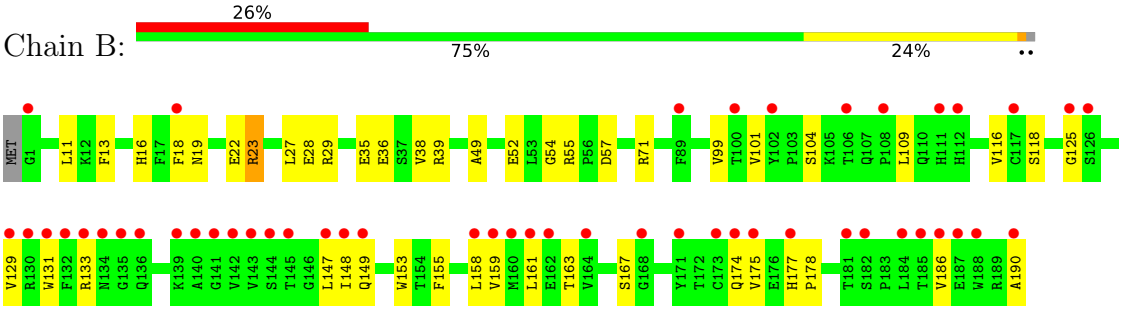
3 Residue-property plots (i)

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.

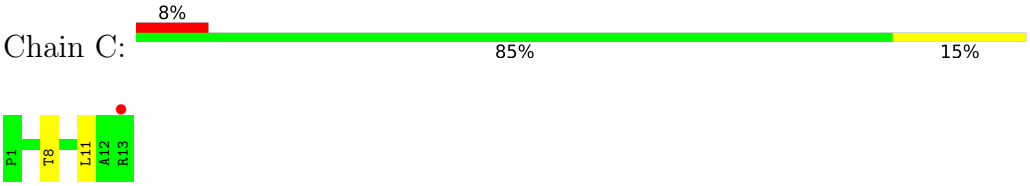
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



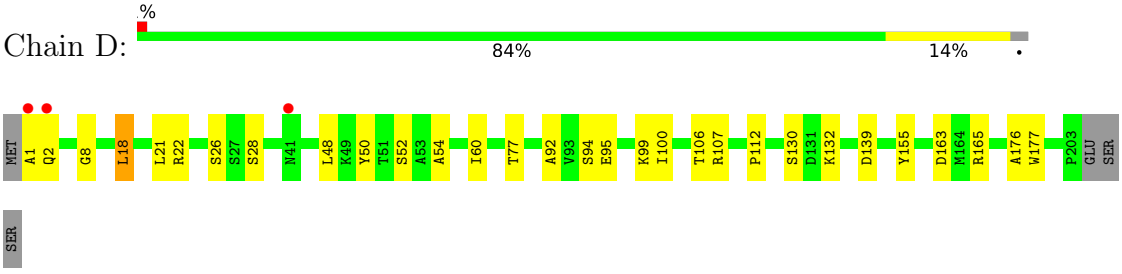
• Molecule 2: HLA class II histocompatibility antigen, DRB1 beta chain



• Molecule 3: Hemagglutinin HA2 chain

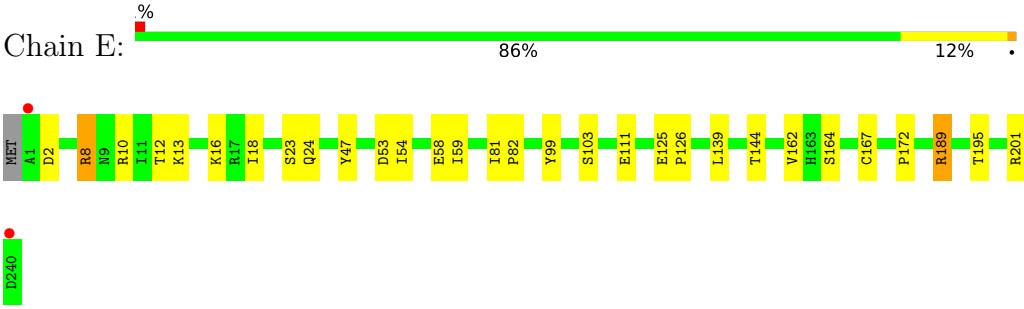


• Molecule 4: T cell receptor alpha chain constant



• Molecule 5: T cell receptor beta constant 1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.61Å 184.82Å 50.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.31 – 1.83 66.31 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.6 (66.31-1.83) 98.6 (66.31-1.83)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.214 0.181 , 0.213	Depositor DCC
R_{free} test set	5364 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: EDO, P4G

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	0.58	0/1518	0.73	1/2070 (0.0%)
2	B	0.54	0/1604	0.74	1/2178 (0.0%)
3	C	0.68	0/111	0.77	0/145
4	D	0.86	0/1688	0.93	3/2289 (0.1%)
5	E	0.89	2/2036 (0.1%)	0.91	2/2765 (0.1%)
All	All	0.75	2/6957 (0.0%)	0.84	7/9447 (0.1%)

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
4	D	0	1
5	E	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	125	GLU	CB-CG	-5.17	1.42	1.52
5	E	125	GLU	CG-CD	5.06	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	48	LEU	CB-CG-CD2	-6.52	99.92	111.00
5	E	189	ARG	CG-CD-NE	6.20	124.83	111.80
2	B	23	ARG	CB-CG-CD	5.89	126.92	111.60
5	E	167	CYS	CA-CB-SG	-5.87	103.43	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	MET	CG-SD-CE	-5.22	91.84	100.20
4	D	18	LEU	CB-CG-CD2	-5.15	102.25	111.00
4	D	139	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	107[A]	ARG	Sidechain
5	E	189	ARG	Sidechain
5	E	8[A]	ARG	Sidechain
5	E	8[B]	ARG	Sidechain

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	1473	0	1407	13	0
2	B	1561	0	1497	35	1
3	C	110	0	127	3	0
4	D	1635	0	1585	30	1
5	E	1967	0	1899	26	0
6	B	8	0	12	5	0
6	C	4	0	6	0	0
6	D	20	0	30	9	0
6	E	28	0	42	11	0
7	D	11	0	18	4	0
7	E	11	0	18	3	0
8	A	38	0	0	0	0
8	B	32	0	0	0	0
8	C	9	0	0	0	0
8	D	148	0	0	1	1
8	E	185	0	0	1	0
All	All	7240	0	6641	101	2

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 7.

All (101) 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)
7:D:306:P4G:H61	5:E:144:THR:HG21	1.53	0.89
5:E:164:SER:HB3	6:E:303:EDO:H22	1.56	0.86
2:B:11:LEU:HD23	3:C:8:THR:HG22	1.59	0.83
5:E:162:VAL:HB	6:E:303:EDO:H21	1.66	0.76
4:D:112:PRO:O	8:D:401:HOH:O	2.05	0.74
2:B:11:LEU:CD2	3:C:8:THR:HG22	2.18	0.72
2:B:129:VAL:HG11	2:B:159:VAL:HG21	1.72	0.71
2:B:11:LEU:HD12	2:B:29:ARG:O	1.92	0.69
2:B:133:ARG:HH21	2:B:163:THR:HG22	1.57	0.69
2:B:39:ARG:HD2	6:B:201:EDO:H11	1.75	0.69
5:E:82:PRO:HD2	7:E:308:P4G:H52	1.75	0.69
5:E:172:PRO:HD3	6:E:307:EDO:H12	1.75	0.66
4:D:22[A]:ARG:HB2	6:D:301:EDO:H11	1.78	0.65
5:E:58:GLU:HG2	5:E:59:ILE:HG23	1.79	0.65
4:D:22[B]:ARG:H	6:D:301:EDO:H11	1.61	0.64
2:B:109:LEU:HD21	2:B:190:ALA:HB1	1.78	0.64
4:D:99:LYS:HD3	5:E:47:TYR:CZ	2.33	0.64
4:D:177:TRP:HE1	7:D:306:P4G:H72	1.63	0.64
4:D:22[A]:ARG:H	6:D:301:EDO:H11	1.61	0.63
2:B:19:ASN:ND2	2:B:22:GLU:OE2	2.36	0.58
2:B:39:ARG:CD	6:B:201:EDO:H11	2.33	0.58
4:D:22[B]:ARG:H	6:D:301:EDO:C1	2.16	0.58
4:D:22[A]:ARG:H	6:D:301:EDO:C1	2.17	0.58
2:B:52:GLU:CD	2:B:55:ARG:HD2	2.24	0.58
4:D:22[B]:ARG:HB2	6:D:301:EDO:H11	1.87	0.57
1:A:36:MET:CE	1:A:63:ILE:HG13	2.35	0.57
5:E:164:SER:H	6:E:303:EDO:H22	1.69	0.57
2:B:16:HIS:HB3	2:B:18:PHE:CZ	2.40	0.56
4:D:22[A]:ARG:HE	6:D:301:EDO:H22	1.71	0.55
2:B:36:GLU:HB3	6:B:202:EDO:H11	1.89	0.55
5:E:8[A]:ARG:NH1	5:E:103:SER:HB3	2.22	0.54
5:E:111:GLU:OE1	7:E:308:P4G:H83	2.08	0.54
5:E:164:SER:CB	6:E:303:EDO:H22	2.34	0.54
4:D:177:TRP:CD1	7:D:306:P4G:H62	2.43	0.54
4:D:92:ALA:HB1	4:D:100:ILE:CG2	2.36	0.54
5:E:8[A]:ARG:H	6:E:302:EDO:H22	1.72	0.54
4:D:1:ALA:HB2	4:D:94:SER:HA	1.89	0.54
5:E:8[B]:ARG:H	6:E:302:EDO:H22	1.72	0.54
4:D:21:LEU:HA	6:D:301:EDO:H21	1.90	0.53
2:B:52:GLU:OE2	2:B:55:ARG:HD2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:VAL:HA	2:B:116:VAL:O	2.08	0.53
5:E:238:ARG:HD3	6:E:304:EDO:H22	1.90	0.52
1:A:73:MET:HG2	3:C:11:LEU:CD1	2.39	0.52
1:A:4:GLU:HG2	2:B:18:PHE:HD1	1.74	0.51
5:E:162:VAL:CB	6:E:303:EDO:H21	2.40	0.50
2:B:35:GLU:HA	6:B:202:EDO:H22	1.92	0.50
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.46	0.50
4:D:18:LEU:HD11	4:D:77[B]:THR:CG2	2.42	0.50
2:B:99:VAL:HG21	2:B:175:VAL:HG11	1.93	0.49
2:B:38[A]:VAL:HG13	2:B:54:GLY:HA3	1.93	0.49
2:B:118:SER:HA	2:B:158:LEU:HD23	1.95	0.49
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.95	0.49
2:B:129:VAL:CG1	2:B:159:VAL:HG21	2.41	0.49
2:B:38[A]:VAL:HG12	2:B:49:ALA:HA	1.94	0.48
2:B:99:VAL:HG12	2:B:186:VAL:HG11	1.95	0.48
5:E:81:ILE:HG21	7:E:308:P4G:H31	1.96	0.48
2:B:147:LEU:HD21	2:B:155:PHE:CD2	2.49	0.48
2:B:36:GLU:H	6:B:202:EDO:C2	2.27	0.47
1:A:36:MET:HE1	1:A:63:ILE:HG13	1.96	0.47
1:A:88:GLU:OE2	1:A:111:LYS:HE3	2.14	0.47
4:D:165:ARG:HA	4:D:165:ARG:HD3	1.65	0.47
4:D:54:ALA:N	6:D:304:EDO:H11	2.31	0.46
1:A:154:LEU:HA	1:A:155:PRO:HD3	1.83	0.46
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.51	0.45
5:E:164:SER:H	6:E:303:EDO:C2	2.30	0.45
4:D:60:ILE:H	4:D:60:ILE:HG12	1.58	0.45
4:D:50:TYR:CZ	4:D:52:SER:HA	2.52	0.45
1:A:129:THR:O	1:A:132:VAL:HG12	2.16	0.45
5:E:201:ARG:HH11	5:E:201:ARG:HG3	1.82	0.45
2:B:125:GLY:O	2:B:147:LEU:HD11	2.17	0.45
5:E:12:THR:HG21	5:E:18:ILE:HG13	1.99	0.44
5:E:16:LYS:HD3	5:E:18:ILE:HD11	1.99	0.44
1:A:119:VAL:HG21	1:A:149:HIS:CD2	2.52	0.44
4:D:165:ARG:HD3	4:D:165:ARG:HH11	1.63	0.44
2:B:18:PHE:CE2	2:B:23:ARG:NH1	2.86	0.44
5:E:126:PRO:HD3	5:E:139:LEU:HG	1.99	0.44
2:B:13:PHE:HD1	2:B:28:GLU:HG2	1.82	0.44
5:E:195:THR:HG23	8:E:560:HOH:O	2.18	0.44
4:D:8:GLY:O	4:D:106:THR:HG23	2.18	0.43
2:B:149:GLN:HG2	2:B:155:PHE:CE2	2.53	0.43
5:E:53:ASP:O	5:E:54:ILE:HD13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:OE2	2:B:71:ARG:NE	2.52	0.43
4:D:1:ALA:HA	4:D:95:GLU:HB2	1.99	0.43
4:D:92:ALA:HB1	4:D:100:ILE:HG23	2.01	0.43
4:D:155:TYR:O	4:D:176:ALA:HA	2.19	0.42
4:D:163:ASP:OD2	4:D:165:ARG:NH1	2.53	0.42
4:D:2:GLN:HB3	4:D:26:SER:O	2.19	0.42
4:D:177:TRP:NE1	7:D:306:P4G:H62	2.35	0.42
4:D:1:ALA:HA	4:D:95:GLU:HG3	2.02	0.41
4:D:1:ALA:CA	4:D:95:GLU:HG3	2.50	0.41
5:E:2:ASP:O	5:E:24:GLN:HA	2.20	0.41
2:B:18:PHE:CD2	2:B:23:ARG:NH1	2.89	0.41
1:A:36:MET:HE2	1:A:63:ILE:HG13	2.03	0.41
2:B:131:TRP:CD1	2:B:161:LEU:HB2	2.56	0.41
2:B:161:LEU:HG	2:B:163:THR:HG23	2.02	0.40
4:D:100:ILE:HD11	5:E:99:TYR:CE1	2.56	0.40
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.94	0.40
1:A:180:PHE:HD1	1:A:181:ASP:N	2.20	0.40
2:B:38[B]:VAL:HG21	2:B:57:ASP:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:SER:O	4:D:130:SER:OG[1_455]	2.09	0.11
8:D:512:HOH:O	8:D:528:HOH:O[2_555]	2.15	0.05

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	177/183 (97%)	176 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	189/191 (99%)	187 (99%)	2 (1%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
4	D	209/207 (101%)	202 (97%)	7 (3%)	0	100	100
5	E	247/241 (102%)	238 (96%)	9 (4%)	0	100	100
All	All	833/835 (100%)	814 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	164/167 (98%)	160 (98%)	4 (2%)	49	32
2	B	172/172 (100%)	168 (98%)	4 (2%)	50	34
3	C	12/12 (100%)	12 (100%)	0	100	100
4	D	189/185 (102%)	187 (99%)	2 (1%)	73	64
5	E	218/210 (104%)	214 (98%)	4 (2%)	59	44
All	All	755/746 (101%)	741 (98%)	14 (2%)	57	42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	164	ARG
1	A	176	LYS
1	A	180	PHE
2	B	27	LEU
2	B	104	SER
2	B	148	ILE
2	B	174	GLN
4	D	28	SER
4	D	132	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	10	ARG
5	E	13	LYS
5	E	23	SER
5	E	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	78	ASN
2	B	92	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)

17 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	EDO	D	302	-	3,3,3	0.66	0	2,2,2	0.23	0
6	EDO	E	304	-	3,3,3	0.45	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	D	301	-	3,3,3	0.48	0	2,2,2	0.33	0
7	P4G	D	306	-	10,10,10	0.64	0	9,9,9	0.83	0
6	EDO	C	101	-	3,3,3	0.68	0	2,2,2	0.25	0
6	EDO	E	306	-	3,3,3	0.44	0	2,2,2	0.21	0
6	EDO	E	303	-	3,3,3	0.74	0	2,2,2	0.78	0
6	EDO	B	201	-	3,3,3	0.44	0	2,2,2	0.52	0
6	EDO	E	305	-	3,3,3	0.59	0	2,2,2	0.03	0
6	EDO	E	307	-	3,3,3	0.46	0	2,2,2	1.04	0
6	EDO	E	302	-	3,3,3	0.64	0	2,2,2	0.46	0
6	EDO	B	202	-	3,3,3	0.43	0	2,2,2	0.31	0
6	EDO	D	304	-	3,3,3	0.32	0	2,2,2	0.85	0
7	P4G	E	308	-	10,10,10	0.58	0	9,9,9	0.82	0
6	EDO	D	305	-	3,3,3	0.46	0	2,2,2	1.17	0
6	EDO	E	301	-	3,3,3	0.62	0	2,2,2	0.33	0
6	EDO	D	303	-	3,3,3	0.50	0	2,2,2	1.54	1 (50%)

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
6	EDO	D	302	-	-	0/1/1/1	-
6	EDO	E	304	-	-	1/1/1/1	-
6	EDO	D	301	-	-	0/1/1/1	-
7	P4G	D	306	-	-	4/8/8/8	-
6	EDO	C	101	-	-	1/1/1/1	-
6	EDO	E	306	-	-	0/1/1/1	-
6	EDO	E	303	-	-	0/1/1/1	-
6	EDO	B	201	-	-	0/1/1/1	-
6	EDO	E	305	-	-	0/1/1/1	-
6	EDO	E	307	-	-	0/1/1/1	-
6	EDO	E	302	-	-	0/1/1/1	-
6	EDO	B	202	-	-	1/1/1/1	-
6	EDO	D	304	-	-	0/1/1/1	-
7	P4G	E	308	-	-	5/8/8/8	-
6	EDO	D	305	-	-	0/1/1/1	-
6	EDO	E	301	-	-	0/1/1/1	-
6	EDO	D	303	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	303	EDO	O1-C1-C2	-2.15	96.44	111.91

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	306	P4G	O2-C3-C4-O3
7	E	308	P4G	C5-C6-O4-C7
6	B	202	EDO	O1-C1-C2-O2
7	E	308	P4G	C1-C2-O2-C3
7	D	306	P4G	C6-C5-O3-C4
7	E	308	P4G	C8-C7-O4-C6
7	D	306	P4G	C3-C4-O3-C5
7	E	308	P4G	O3-C5-C6-O4
6	E	304	EDO	O1-C1-C2-O2
7	E	308	P4G	O2-C3-C4-O3
7	D	306	P4G	O3-C5-C6-O4
6	C	101	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	304	EDO	1	0
6	D	301	EDO	8	0
7	D	306	P4G	4	0
6	E	303	EDO	6	0
6	B	201	EDO	2	0
6	E	307	EDO	1	0
6	E	302	EDO	3	0
6	B	202	EDO	3	0
6	D	304	EDO	1	0
7	E	308	P4G	3	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^{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	179/183 (97%)	0.42	18 (10%) 7 6	34, 59, 109, 140	0
2	B	190/191 (99%)	1.06	50 (26%) 0 0	37, 74, 111, 131	0
3	C	13/13 (100%)	0.20	1 (7%) 13 12	38, 41, 56, 81	0
4	D	203/207 (98%)	0.25	3 (1%) 73 73	19, 34, 69, 93	0
5	E	240/241 (99%)	0.06	2 (0%) 86 86	20, 35, 60, 97	0
All	All	825/835 (98%)	0.42	74 (8%) 9 8	19, 46, 100, 140	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	PHE	6.4
1	A	180	PHE	6.0
4	D	1	ALA	5.8
1	A	99	LEU	5.4
2	B	112	HIS	5.0
2	B	160	MET	4.9
1	A	100	ARG	4.8
2	B	134	ASN	4.6
2	B	106	THR	4.4
2	B	173	CYS	4.3
2	B	142	VAL	4.3
2	B	186	VAL	4.3
1	A	181	ASP	3.9
2	B	161	LEU	3.8
2	B	139	LYS	3.7
2	B	181	THR	3.6
2	B	111	HIS	3.6
2	B	182	SER	3.6
2	B	144	SER	3.5
2	B	158	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	3.5
1	A	154	LEU	3.5
5	E	240	ASP	3.4
2	B	102	TYR	3.4
1	A	122	LEU	3.3
2	B	159	VAL	3.3
2	B	140	ALA	3.3
2	B	130	ARG	3.3
2	B	18	PHE	3.2
1	A	158	GLU	3.2
2	B	129	VAL	3.2
2	B	108	PRO	3.1
2	B	171	TYR	3.1
1	A	97	VAL	3.1
2	B	143	VAL	3.1
2	B	145	THR	3.1
2	B	190	ALA	3.0
5	E	1	ALA	3.0
2	B	117	CYS	3.0
1	A	46	GLU	2.9
1	A	3	GLU	2.9
2	B	131	TRP	2.9
2	B	175	VAL	2.9
2	B	1	GLY	2.9
2	B	141	GLY	2.8
2	B	100	THR	2.8
2	B	184	LEU	2.8
2	B	126	SER	2.7
2	B	136	GLN	2.7
2	B	185	THR	2.7
2	B	164	VAL	2.6
3	C	13	ARG	2.6
1	A	98	GLU	2.6
2	B	125	GLY	2.6
1	A	101	GLU	2.6
2	B	147	LEU	2.5
2	B	135	GLY	2.5
2	B	148	ILE	2.5
2	B	89	PHE	2.5
4	D	2	GLN	2.5
1	A	94	ASN	2.4
2	B	174	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	GLU	2.4
2	B	177	HIS	2.3
2	B	168	GLY	2.2
1	A	157	THR	2.2
2	B	133	ARG	2.2
1	A	153	PHE	2.2
2	B	162	GLU	2.1
2	B	187	GLU	2.1
4	D	41	ASN	2.1
2	B	149	GLN	2.1
2	B	188	TRP	2.0
1	A	124	ASN	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
7	P4G	D	306	11/11	0.76	0.21	39,63,73,75	0
7	P4G	E	308	11/11	0.81	0.35	41,62,71,71	0
6	EDO	E	303	4/4	0.82	0.18	35,40,42,53	0
6	EDO	E	306	4/4	0.85	0.47	63,67,68,75	0
6	EDO	E	305	4/4	0.86	0.28	57,60,75,79	0
6	EDO	E	302	4/4	0.88	0.16	44,46,51,55	0
6	EDO	E	301	4/4	0.90	0.09	46,58,61,65	0
6	EDO	B	202	4/4	0.91	0.36	60,60,63,65	0
6	EDO	E	307	4/4	0.92	0.37	45,50,54,62	0
6	EDO	E	304	4/4	0.93	0.19	55,56,60,73	0
6	EDO	D	304	4/4	0.93	0.19	38,47,59,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	302	4/4	0.93	0.13	36,44,46,48	0
6	EDO	D	303	4/4	0.94	0.23	35,44,49,59	0
6	EDO	D	305	4/4	0.95	0.09	36,48,53,61	0
6	EDO	D	301	4/4	0.95	0.15	27,41,46,53	0
6	EDO	C	101	4/4	0.96	0.11	35,35,37,45	0
6	EDO	B	201	4/4	0.97	0.26	43,51,53,58	0

6.5 Other polymers

There are no such residues in this entry.