



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 07:19 pm BST

PDB ID : 7Q99
Title : MHC Class I A02 Allele presenting NLSALGIFST, in complex with Mel5 TCR
Authors : Rizkallah, P.J.; Sewell, A.K.; Wall, A.; Fuller, A.
Deposited on : 2021-11-12
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

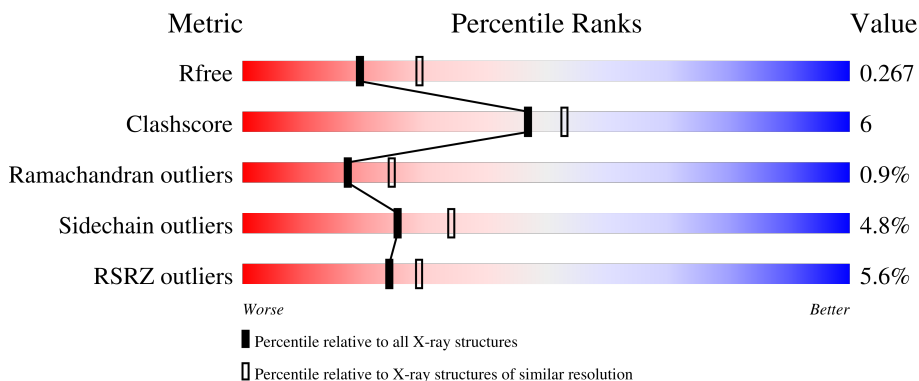
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	276	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
2	B	100	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
3	C	10	<div style="display: flex; align-items: center;"> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
4	D	198	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
5	E	244	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6664 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2253	1408	410	426	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	72	46	11	15	0	0	0

- Molecule 4 is a protein called Mel5 Human TCR, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	198	1531	953	252	318	8	0	0	0

- Molecule 5 is a protein called Mel5 Human TCR, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	244	1926	1221	330	370	5	0	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

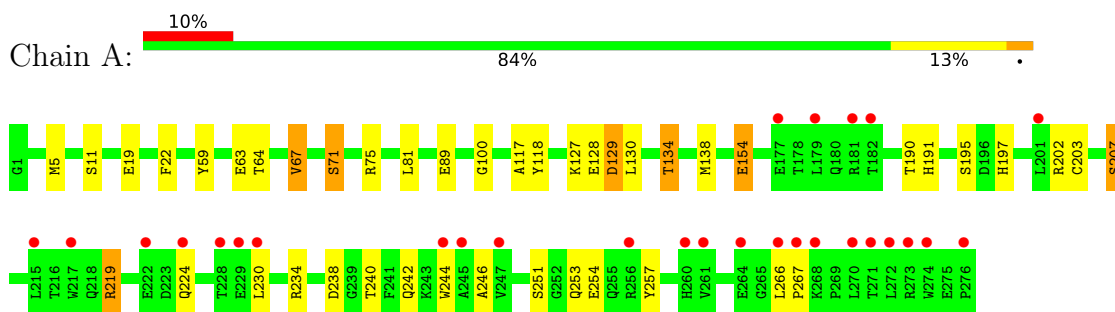
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	15	Total O 15 15	0	0
7	B	2	Total O 2 2	0	0
7	D	11	Total O 11 11	0	0
7	E	9	Total O 9 9	0	0

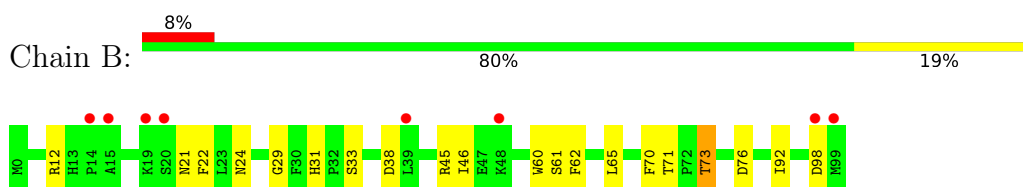
3 Residue-property plots [i](#)

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.

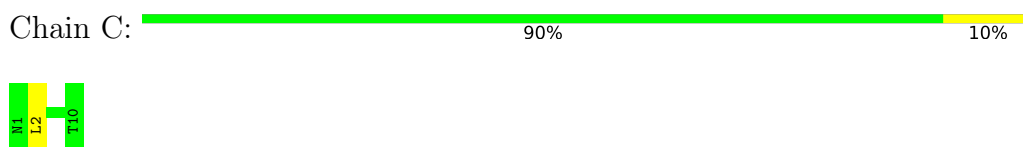
- Molecule 1: MHC class I antigen



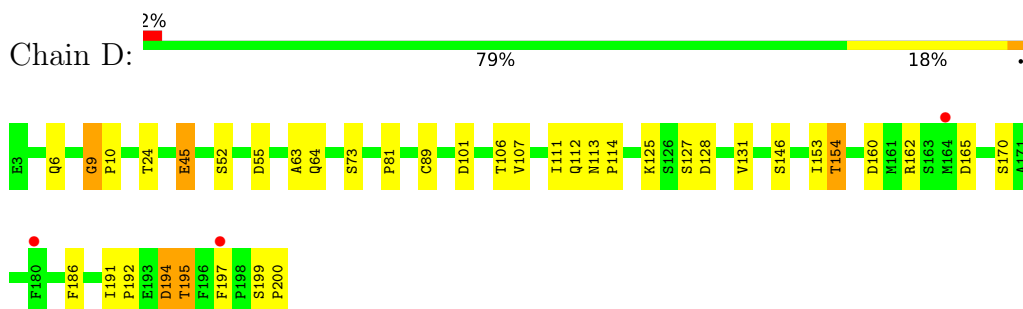
- Molecule 2: Beta-2-microglobulin



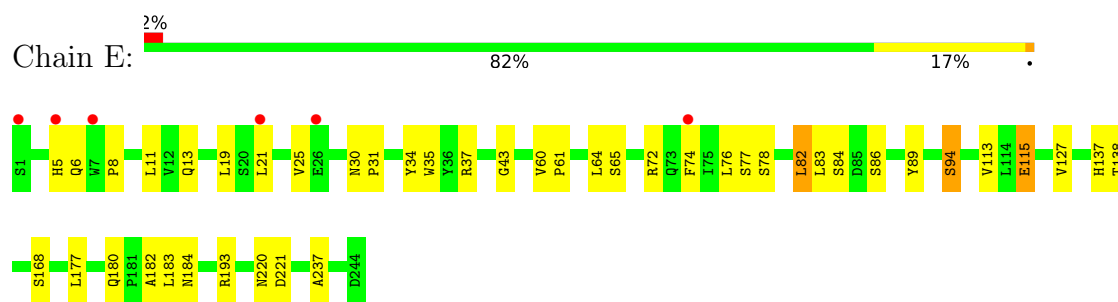
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR



- Molecule 4: Mel5 Human TCR, alpha chain



- Molecule 5: Mel5 Human TCR, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.28Å 121.28Å 81.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.64 – 2.55 60.64 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (60.64-2.55) 99.0 (60.64-2.55)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.218 , 0.272 0.219 , 0.267	Depositor DCC
R_{free} test set	1905 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtrriage
Anisotropy	0.450	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6664	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: EDO

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	0.78	1/2319 (0.0%)	0.83	0/3149
2	B	0.75	0/860	0.83	0/1162
3	C	0.88	0/72	0.93	0/95
4	D	0.75	1/1564 (0.1%)	0.83	0/2122
5	E	0.71	0/1979	0.81	0/2698
All	All	0.75	2/6794 (0.0%)	0.83	0/9226

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	45	GLU	CD-OE1	5.76	1.31	1.25
1	A	89	GLU	CD-OE1	5.67	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	186	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	0	2103	25	0
2	B	837	0	803	10	0
3	C	72	0	75	1	0
4	D	1531	0	1439	23	0
5	E	1926	0	1845	28	0
6	A	8	0	12	0	0
7	A	15	0	0	0	0
7	B	2	0	0	0	0
7	D	11	0	0	0	0
7	E	9	0	0	0	0
All	All	6664	0	6277	80	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 6.

All (80) 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)
4:D:131:VAL:HG22	4:D:174:TRP:HB3	1.64	0.80
4:D:6:GLN:HE22	4:D:89:CYS:H	1.43	0.67
5:E:37:ARG:HD2	5:E:89:TYR:CZ	2.30	0.66
5:E:34:TYR:HE1	5:E:94:SER:HB3	1.62	0.64
1:A:127:LYS:HE2	1:A:134:THR:HG22	1.79	0.63
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.34	0.63
4:D:195:THR:HG21	4:D:197:PHE:CZ	2.34	0.62
2:B:38:ASP:OD1	2:B:45:ARG:HD2	2.00	0.62
5:E:19:LEU:O	5:E:77:SER:HA	2.00	0.62
4:D:191:ILE:HG23	4:D:194:ASP:OD2	1.99	0.61
1:A:191:HIS:NE2	1:A:254:GLU:OE2	2.34	0.61
1:A:127:LYS:CE	1:A:134:THR:HG22	2.30	0.60
4:D:194:ASP:N	4:D:194:ASP:OD1	2.32	0.60
1:A:238:ASP:HB3	2:B:12:ARG:HD3	1.85	0.57
5:E:37:ARG:HD2	5:E:89:TYR:CE1	2.39	0.57
2:B:29:GLY:HA2	2:B:61:SER:OG	2.05	0.57
5:E:177:LEU:C	5:E:177:LEU:HD12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:PRO:HG2	5:E:11:LEU:HD21	1.86	0.56
2:B:73:THR:HG22	2:B:76:ASP:OD2	2.06	0.55
4:D:199:SER:N	4:D:200:PRO:CD	2.69	0.55
4:D:197:PHE:HZ	5:E:137:HIS:CD2	2.23	0.55
4:D:131:VAL:HG22	4:D:174:TRP:CB	2.37	0.54
5:E:82:LEU:HD12	5:E:82:LEU:H	1.72	0.54
4:D:81:PRO:HA	4:D:107:VAL:HB	1.90	0.54
5:E:5:HIS:CD2	5:E:6:GLN:H	2.26	0.54
4:D:55:ASP:OD1	4:D:64:GLN:HG3	2.09	0.52
1:A:219:ARG:HG2	1:A:257:TYR:CE2	2.44	0.52
5:E:82:LEU:HD12	5:E:82:LEU:N	2.25	0.52
2:B:21:ASN:OD1	2:B:22:PHE:N	2.36	0.52
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.92	0.52
1:A:190:THR:HG21	2:B:98:ASP:OD1	2.11	0.50
5:E:30:ASN:N	5:E:31:PRO:CD	2.75	0.50
4:D:154:THR:HG23	4:D:172:VAL:O	2.12	0.49
5:E:127:VAL:HG13	5:E:237:ALA:HB3	1.94	0.49
5:E:180:GLN:O	5:E:182:ALA:N	2.45	0.49
1:A:202:ARG:HG3	1:A:246:ALA:HB2	1.94	0.49
4:D:101:ASP:HA	5:E:43:GLY:HA3	1.94	0.49
5:E:25:VAL:O	5:E:72:ARG:HD2	2.13	0.49
4:D:160:ASP:O	4:D:162:ARG:NH2	2.46	0.49
1:A:251:SER:O	1:A:254:GLU:HG2	2.13	0.48
4:D:191:ILE:CG2	4:D:194:ASP:OD2	2.61	0.48
5:E:21:LEU:HD12	5:E:76:LEU:HD23	1.95	0.48
1:A:203:CYS:O	1:A:244:TRP:HA	2.13	0.47
5:E:220:ASN:OD1	5:E:220:ASN:N	2.46	0.47
5:E:13:GLN:O	5:E:113:VAL:HA	2.15	0.47
5:E:35:TRP:CD1	5:E:74:PHE:CE2	3.04	0.46
1:A:64:THR:O	1:A:67:VAL:HG12	2.15	0.46
4:D:195:THR:HB	4:D:197:PHE:CE2	2.51	0.46
4:D:63:ALA:HA	4:D:73:SER:O	2.16	0.45
5:E:37:ARG:NH2	5:E:84:SER:O	2.50	0.45
4:D:162:ARG:HD2	4:D:162:ARG:H	1.82	0.45
4:D:199:SER:N	4:D:200:PRO:HD2	2.32	0.45
4:D:112:GLN:HG3	4:D:113:ASN:OD1	2.18	0.44
5:E:34:TYR:CE1	5:E:94:SER:HB3	2.49	0.44
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.53	0.43
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.18	0.43
1:A:22:PHE:CG	1:A:71:SER:HB2	2.53	0.43
1:A:19:GLU:OE1	1:A:75:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:OE2	1:A:154:GLU:N	2.52	0.43
1:A:63:GLU:OE1	3:C:2:LEU:HD23	2.19	0.42
5:E:83:LEU:HD21	5:E:115:GLU:HG2	2.02	0.42
4:D:146:SER:HB2	4:D:153:ILE:HD12	2.01	0.42
1:A:230:LEU:HD23	1:A:230:LEU:H	1.84	0.42
2:B:73:THR:CG2	2:B:76:ASP:OD2	2.67	0.42
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.68	0.42
1:A:195:SER:HB2	1:A:197:HIS:H	1.83	0.42
5:E:25:VAL:O	5:E:72:ARG:HB3	2.20	0.42
5:E:60:VAL:CG2	5:E:61:PRO:HD2	2.50	0.41
1:A:266:LEU:HA	1:A:267:PRO:HD2	1.89	0.41
1:A:128:GLU:C	1:A:130:LEU:H	2.24	0.41
4:D:9:GLY:HA3	4:D:10:PRO:HA	1.94	0.41
1:A:5:MET:O	1:A:100:GLY:HA3	2.21	0.41
1:A:207:SER:HA	1:A:240:THR:CB	2.51	0.41
4:D:162:ARG:NH2	5:E:168:SER:HA	2.36	0.41
5:E:8:PRO:CG	5:E:11:LEU:HD21	2.51	0.41
5:E:64:LEU:HD23	5:E:78:SER:HB2	2.03	0.41
5:E:180:GLN:HB3	5:E:183:LEU:HD23	2.03	0.41
4:D:111:ILE:O	4:D:114:PRO:HD3	2.21	0.40
1:A:59:TYR:O	1:A:63:GLU:HG2	2.20	0.40
2:B:31:HIS:CE1	2:B:62:PHE:CE2	3.09	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	274/276 (99%)	250 (91%)	21 (8%)	3 (1%)	14	19
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	196/198 (99%)	170 (87%)	22 (11%)	4 (2%)	7	8
5	E	242/244 (99%)	223 (92%)	19 (8%)	0	100	100
All	All	818/828 (99%)	744 (91%)	67 (8%)	7 (1%)	17	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
4	D	165	ASP
4	D	192	PRO
4	D	128	ASP
1	A	129	ASP
1	A	138	MET
4	D	9	GLY

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	232/232 (100%)	223 (96%)	9 (4%)	32	44
2	B	95/95 (100%)	89 (94%)	6 (6%)	18	23
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	176/176 (100%)	165 (94%)	11 (6%)	18	23
5	E	211/211 (100%)	202 (96%)	9 (4%)	29	39
All	All	722/722 (100%)	687 (95%)	35 (5%)	25	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	67	VAL
1	A	71	SER
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	134	THR
1	A	154	GLU
1	A	207	SER
1	A	219	ARG
1	A	253	GLN
2	B	33	SER
2	B	46	ILE
2	B	70	PHE
2	B	71	THR
2	B	73	THR
2	B	92	ILE
4	D	24	THR
4	D	45	GLU
4	D	52	SER
4	D	106	THR
4	D	125	LYS
4	D	127	SER
4	D	154	THR
4	D	170	SER
4	D	176	ASN
4	D	194	ASP
4	D	195	THR
5	E	65	SER
5	E	82	LEU
5	E	86	SER
5	E	94	SER
5	E	115	GLU
5	E	138	THR
5	E	184	ASN
5	E	193	ARG
5	E	221	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	86	ASN
1	A	141	GLN
1	A	174	ASN
1	A	180	GLN
1	A	188	HIS
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	242	GLN
2	B	31	HIS
2	B	83	ASN
4	D	6	GLN
4	D	38	GLN
5	E	5	HIS
5	E	38	GLN
5	E	55	GLN
5	E	119	ASN
5	E	137	HIS
5	E	213	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](#)

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	EDO	A	301	-	3,3,3	0.10	0	2,2,2	0.14	0
6	EDO	A	302	-	3,3,3	0.08	0	2,2,2	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
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	A	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	EDO	O1-C1-C2-O2
6	A	302	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	276/276 (100%)	0.72	28 (10%) 7 8	49, 71, 125, 147	0
2	B	100/100 (100%)	0.73	8 (8%) 12 15	48, 79, 112, 123	0
3	C	10/10 (100%)	0.63	0 100 100	51, 58, 65, 67	0
4	D	198/198 (100%)	0.47	4 (2%) 65 72	48, 70, 133, 150	0
5	E	244/244 (100%)	0.48	6 (2%) 57 63	51, 72, 106, 127	0
All	All	828/828 (100%)	0.59	46 (5%) 24 29	48, 72, 121, 150	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	4.9
1	A	274	TRP	4.8
1	A	228	THR	4.4
1	A	229	GLU	4.3
5	E	7	TRP	3.8
4	D	180	PHE	3.7
1	A	270	LEU	3.5
1	A	272	LEU	3.5
2	B	99	MET	3.2
2	B	14	PRO	3.2
1	A	268	LYS	3.1
1	A	201	LEU	3.0
5	E	74	PHE	3.0
1	A	224	GLN	3.0
1	A	256	ARG	3.0
1	A	271	THR	2.9
1	A	266	LEU	2.9
1	A	247	VAL	2.8
2	B	15	ALA	2.8
1	A	261	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	2.7
1	A	260	HIS	2.6
1	A	182	THR	2.5
4	D	176	ASN	2.5
1	A	245	ALA	2.5
1	A	217	TRP	2.5
5	E	5	HIS	2.5
1	A	273	ARG	2.5
4	D	197	PHE	2.5
1	A	179	LEU	2.4
2	B	98	ASP	2.4
2	B	19	LYS	2.4
1	A	244	TRP	2.4
1	A	230	LEU	2.4
2	B	48	LYS	2.3
4	D	164	MET	2.3
1	A	181	ARG	2.3
1	A	215	LEU	2.3
5	E	26	GLU	2.2
2	B	39	LEU	2.2
1	A	264	GLU	2.2
5	E	1	SER	2.2
1	A	222	GLU	2.1
5	E	21	LEU	2.1
1	A	267	PRO	2.0
2	B	20	SER	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, 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(\AA^2)	Q<0.9
6	EDO	A	301	4/4	0.82	0.18	76,76,77,79	0
6	EDO	A	302	4/4	0.83	0.12	87,88,90,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.