



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:34 AM UTC

PDB ID : 7NMF / pdb_00007nmf
Title : Human MHC Class I, A24 Allele presenting QLPRLFPLL, Complex with 4C6 TCR, monoclinic form
Authors : Rizkallah, P.J.; Sewell, A.K.; Cole, D.K.; Wall, A.
Deposited on : 2021-02-23
Resolution : 2.98 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

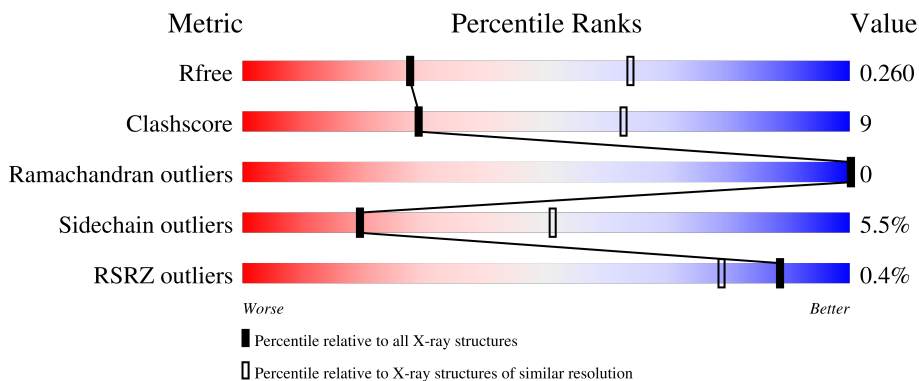
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	 73% 25% .
2	B	100	 82% 14% .
3	C	9	 44% 56%
4	D	194	 2% 78% 20% .
5	E	240	 80% 20% .

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
7	EDO	D	201	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6682 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	2238	1392	405	431	10	0	0	0

- Molecule 2 is a protein called Human MHC Class I, 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 GLN-LEU-PRO-ARG-LEU-PHE-PRO-LEU-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	78	54	13	11	0	0	0

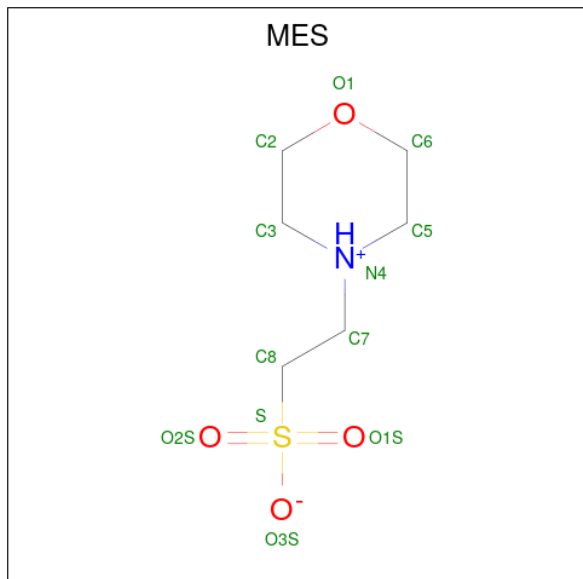
- Molecule 4 is a protein called Human T-cell Receptor 4C6, alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	194	1515	944	249	313	9	0	0	0

- Molecule 5 is a protein called Human T-cell Receptor 4C6, beta Chain.

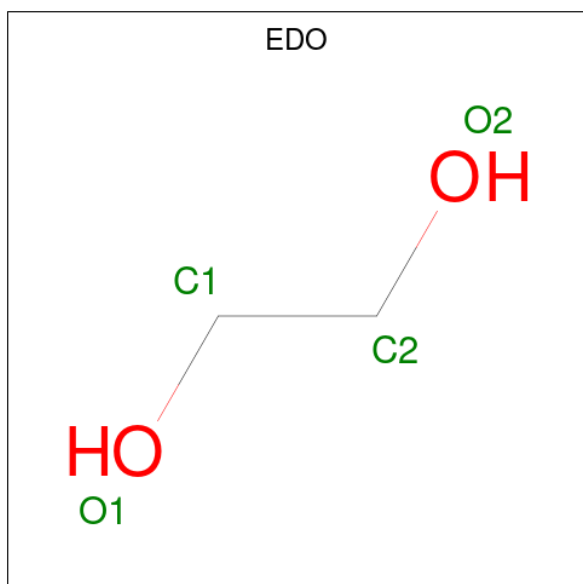
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	240	1943	1218	347	372	6	0	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	12	6	1	4	1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	4	2	2	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		

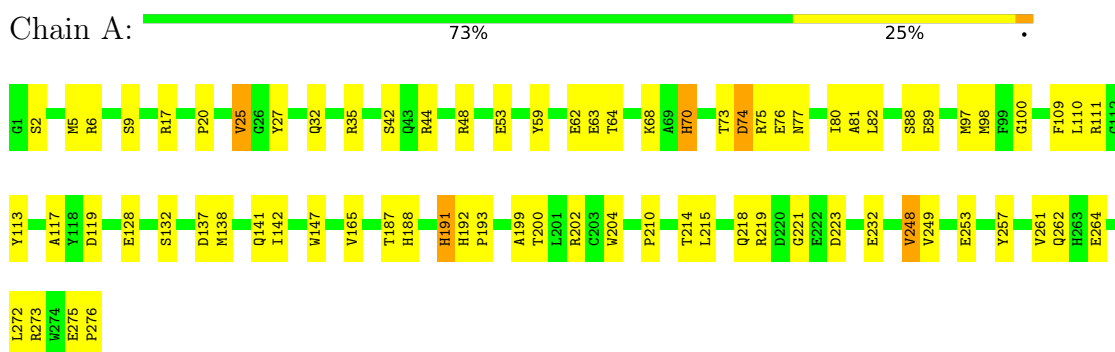
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	12	Total	O	0	0
			12	12		
9	B	4	Total	O	0	0
			4	4		
9	D	17	Total	O	0	0
			17	17		
9	E	12	Total	O	0	0
			12	12		

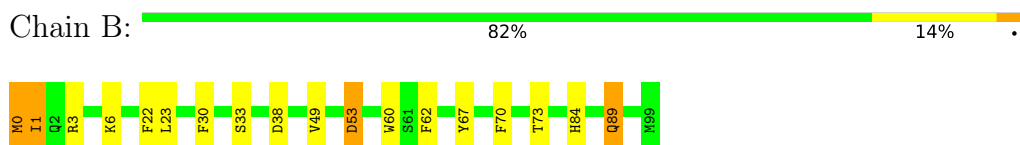
3 Residue-property plots

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.

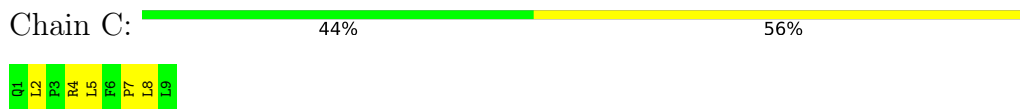
- Molecule 1: MHC class I antigen



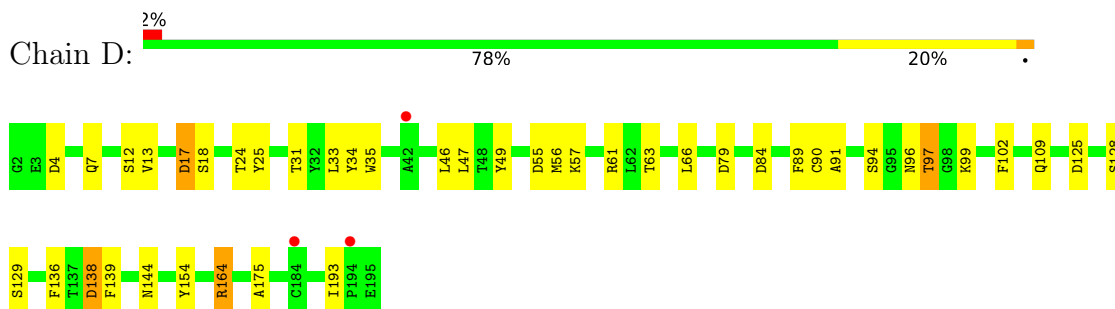
- Molecule 2: Human MHC Class I, beta 2 microglobulin




- Molecule 3: GLN-LEU-PRO-ARG-LEU-PHE-PRO-LEU-LEU

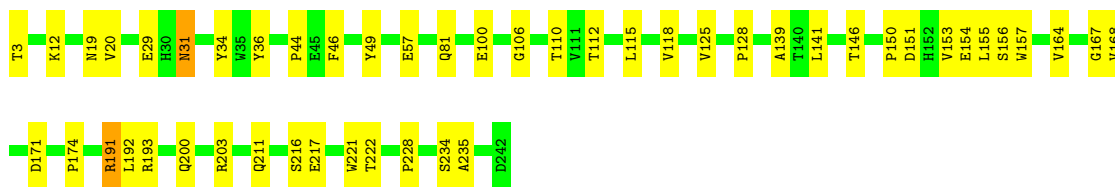


- Molecule 4: Human T-cell Receptor 4C6, alpha Chain



- Molecule 5: Human T-cell Receptor 4C6, beta Chain

Chain E:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.38Å 72.25Å 114.84Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	60.15 – 2.98 60.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	96.4 (60.15-2.98) 96.4 (60.15-2.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.259 0.185 , 0.260	Depositor DCC
R_{free} test set	980 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtrriage
Anisotropy	0.283	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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, EDO, MES

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	1.17	2/2299 (0.1%)	1.42	5/3116 (0.2%)
2	B	1.12	1/860 (0.1%)	1.24	0/1162
3	C	1.07	1/80 (1.2%)	1.17	0/107
4	D	1.17	1/1542 (0.1%)	1.41	7/2087 (0.3%)
5	E	1.13	0/1996	1.36	1/2712 (0.0%)
All	All	1.15	5/6777 (0.1%)	1.38	13/9184 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	HIS	CE1-NE2	6.86	1.39	1.32
1	A	20	PRO	C-O	-6.74	1.15	1.23
3	C	5	LEU	C-O	5.23	1.30	1.23
4	D	97	THR	C-O	5.19	1.31	1.23
2	B	38	ASP	C-O	-5.01	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	129	SER	CA-C-N	6.32	129.07	120.54
4	D	129	SER	C-N-CA	6.32	129.07	120.54
4	D	17	ASP	CA-CB-CG	6.24	118.84	112.60
4	D	96	ASN	CB-CA-C	6.11	119.33	109.07
4	D	55	ASP	CB-CA-C	-5.45	101.86	110.86
1	A	210	PRO	CA-C-N	5.45	128.13	120.28
1	A	210	PRO	C-N-CA	5.45	128.13	120.28
5	E	106	GLY	CA-C-O	-5.32	117.98	122.29
1	A	62	GLU	CA-C-N	5.15	127.61	120.29
1	A	62	GLU	C-N-CA	5.15	127.61	120.29
4	D	96	ASN	N-CA-C	-5.07	107.48	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	138	ASP	N-CA-C	-5.02	107.10	113.23
1	A	142	ILE	N-CA-C	-5.00	105.83	110.53

There are no chirality outliers.

There are no planarity outliers.

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	2238	0	2095	49	0
2	B	837	0	803	14	0
3	C	78	0	90	5	0
4	D	1515	0	1452	28	0
5	E	1943	0	1838	28	0
6	A	12	0	13	3	0
7	D	4	0	6	4	0
8	E	10	0	0	0	0
9	A	12	0	0	1	0
9	B	4	0	0	1	0
9	D	17	0	0	0	0
9	E	12	0	0	0	0
All	All	6682	0	6297	113	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 9.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HD3	1:A:48:ARG:HD3	1.61	0.82
1:A:35:ARG:CD	1:A:48:ARG:HD3	2.16	0.75
1:A:59:TYR:O	1:A:63:GLU:HG2	1.93	0.69
1:A:219:ARG:HB3	1:A:257:TYR:CD2	2.28	0.68
1:A:187:THR:HB	1:A:272:LEU:HD11	1.74	0.67
5:E:12:LYS:HG2	5:E:20:VAL:HG21	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:ASP:OD1	5:E:174:PRO:HG2	1.95	0.66
1:A:218:GLN:HA	1:A:223:ASP:HB3	1.80	0.64
4:D:97:THR:HG22	5:E:49:TYR:CE2	2.33	0.64
1:A:35:ARG:HH11	1:A:48:ARG:HH11	1.47	0.62
1:A:193:PRO:HA	1:A:199:ALA:HA	1.81	0.62
5:E:151:ASP:CG	5:E:174:PRO:HG2	2.25	0.61
2:B:84:HIS:O	9:B:101:HOH:O	2.16	0.61
4:D:125:ASP:HB3	4:D:128:SER:O	2.03	0.58
4:D:34:TYR:OH	5:E:100:GLU:HA	2.02	0.58
4:D:34:TYR:CD1	4:D:49:TYR:HB3	2.38	0.58
5:E:125:VAL:HG23	5:E:235:ALA:HB3	1.86	0.57
5:E:155:LEU:C	5:E:155:LEU:HD23	2.28	0.57
1:A:35:ARG:HD2	2:B:53:ASP:OD2	2.05	0.56
1:A:214:THR:OG1	1:A:262:GLN:HB2	2.06	0.56
1:A:187:THR:HA	1:A:204:TRP:O	2.05	0.56
1:A:119:ASP:HB3	2:B:0:MET:HA	1.88	0.56
1:A:98:MET:SD	1:A:98:MET:C	2.89	0.55
3:C:8:LEU:HD12	5:E:31:ASN:HB2	1.87	0.54
4:D:61:ARG:NH2	4:D:79:ASP:O	2.41	0.54
5:E:128:PRO:HG3	5:E:139:ALA:HB1	1.89	0.53
5:E:153:VAL:HA	5:E:211:GLN:O	2.09	0.53
1:A:147:TRP:CZ2	3:C:7:PRO:HB2	2.45	0.52
4:D:7:GLN:HE22	4:D:89:PHE:HA	1.75	0.52
2:B:3:ARG:O	2:B:30:PHE:HA	2.10	0.52
1:A:9:SER:HB2	1:A:70:HIS:CE1	2.45	0.51
1:A:249:VAL:HG12	1:A:257:TYR:CZ	2.46	0.51
5:E:203:ARG:HH11	5:E:203:ARG:HB2	1.76	0.50
5:E:31:ASN:H	5:E:31:ASN:HD22	1.61	0.49
4:D:61:ARG:HH12	4:D:84:ASP:CG	2.21	0.49
1:A:137:ASP:OD1	1:A:137:ASP:C	2.55	0.48
2:B:22:PHE:C	2:B:70:PHE:HE1	2.21	0.48
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.82	0.48
3:C:4:ARG:HB2	7:D:201:EDO:C2	2.44	0.47
3:C:8:LEU:HD12	5:E:31:ASN:CB	2.44	0.47
4:D:13:VAL:HG22	4:D:17:ASP:HB2	1.95	0.47
1:A:81:ALA:O	1:A:82:LEU:C	2.57	0.47
1:A:53:GLU:OE1	6:A:301:MES:H61	2.14	0.47
4:D:144:ASN:HB3	4:D:193:ILE:HG12	1.97	0.47
4:D:154:TYR:O	4:D:175:ALA:HA	2.14	0.47
5:E:203:ARG:HB2	5:E:203:ARG:NH1	2.29	0.47
1:A:74:ASP:HA	1:A:77:ASN:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:O	1:A:80:ILE:HG13	2.15	0.46
1:A:192:HIS:HE1	1:A:202:ARG:HE	1.62	0.46
1:A:109:PHE:HD2	1:A:165:VAL:CG2	2.27	0.46
1:A:188:HIS:O	1:A:204:TRP:HB2	2.15	0.46
4:D:138:ASP:OD2	5:E:193:ARG:NH2	2.41	0.46
1:A:219:ARG:O	1:A:219:ARG:HG3	2.15	0.46
1:A:248:VAL:C	1:A:249:VAL:HG13	2.41	0.46
1:A:191:HIS:HA	1:A:200:THR:O	2.16	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.51	0.46
6:A:301:MES:H32	9:A:412:HOH:O	2.16	0.45
1:A:275:GLU:O	1:A:276:PRO:C	2.58	0.45
4:D:94:SER:HB3	4:D:99:LYS:HE3	1.99	0.45
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.48	0.44
5:E:168:VAL:HA	5:E:191:ARG:O	2.17	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.17	0.44
1:A:232:GLU:OE1	2:B:6:LYS:HD3	2.17	0.44
2:B:22:PHE:C	2:B:70:PHE:CE1	2.96	0.44
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.52	0.44
1:A:5:MET:O	1:A:100:GLY:HA3	2.17	0.44
5:E:19:ASN:OD1	5:E:81:GLN:HA	2.17	0.44
1:A:25:VAL:CG1	1:A:27:TYR:CE2	3.00	0.44
4:D:144:ASN:HB3	4:D:193:ILE:CG1	2.48	0.44
1:A:25:VAL:HG13	1:A:32:GLN:HG3	2.00	0.44
1:A:138:MET:HA	1:A:141:GLN:HG3	1.99	0.44
5:E:110:THR:HG21	5:E:150:PRO:HB3	2.00	0.43
1:A:42:SER:O	1:A:44:ARG:HG3	2.18	0.43
1:A:64:THR:HG22	1:A:68:LYS:HD2	1.99	0.43
4:D:91:ALA:HB2	4:D:102:PHE:CD1	2.53	0.43
4:D:144:ASN:O	4:D:193:ILE:HG12	2.19	0.43
4:D:31:THR:HG21	7:D:201:EDO:H11	2.00	0.43
4:D:102:PHE:CD2	5:E:44:PRO:HD2	2.54	0.43
2:B:1:ILE:HD13	2:B:1:ILE:HA	1.93	0.43
5:E:171:ASP:OD1	5:E:191:ARG:NH1	2.51	0.43
4:D:33:LEU:HD13	4:D:66:LEU:HD13	1.99	0.43
5:E:217:GLU:H	5:E:217:GLU:CD	2.26	0.43
4:D:25:TYR:CD2	4:D:33:LEU:HD21	2.54	0.43
1:A:219:ARG:HB3	1:A:257:TYR:CE2	2.54	0.42
2:B:0:MET:HE3	2:B:0:MET:HB2	1.96	0.42
3:C:4:ARG:HB2	7:D:201:EDO:H22	2.01	0.42
5:E:167:GLY:O	5:E:192:LEU:HD12	2.20	0.42
1:A:48:ARG:HA	6:A:301:MES:H22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:136:PHE:O	4:D:139:PHE:HE2	2.02	0.42
1:A:111:ARG:HD3	1:A:128:GLU:OE2	2.20	0.42
4:D:46:LEU:HD23	4:D:46:LEU:C	2.44	0.42
5:E:115:LEU:O	5:E:221:TRP:HZ3	2.02	0.42
5:E:118:VAL:HG12	5:E:228:PRO:HB2	2.00	0.42
1:A:218:GLN:HB2	1:A:221:GLY:O	2.20	0.42
4:D:56:MET:HG2	4:D:57:LYS:N	2.35	0.42
4:D:31:THR:CG2	7:D:201:EDO:H11	2.50	0.42
1:A:64:THR:O	1:A:68:LYS:HB2	2.20	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.41
4:D:12:SER:OG	4:D:109:GLN:NE2	2.53	0.41
1:A:9:SER:HB3	1:A:97:MET:HG2	2.03	0.41
5:E:34:TYR:N	5:E:34:TYR:CD1	2.89	0.41
5:E:157:TRP:HB2	5:E:164:VAL:CG2	2.50	0.41
1:A:32:GLN:HE21	1:A:48:ARG:HG3	1.85	0.41
2:B:89:GLN:HE21	2:B:89:GLN:HB2	1.63	0.41
1:A:215:LEU:HD22	1:A:261:VAL:HG22	2.03	0.40
1:A:219:ARG:HA	1:A:257:TYR:HA	2.01	0.40
5:E:141:LEU:N	5:E:141:LEU:HD12	2.36	0.40
1:A:218:GLN:O	1:A:257:TYR:HA	2.22	0.40
4:D:46:LEU:HD23	4:D:47:LEU:N	2.36	0.40
4:D:164:ARG:HA	4:D:164:ARG:NE	2.36	0.40
5:E:36:TYR:CD2	5:E:46:PHE:HA	2.56	0.40
4:D:35:TRP:CZ3	4:D:90:CYS:HB3	2.55	0.40
4:D:47:LEU:HD12	4:D:47:LEU:HA	1.87	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%)	259 (94%)	15 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	192/194 (99%)	184 (96%)	8 (4%)	0	100	100
5	E	238/240 (99%)	225 (94%)	13 (6%)	0	100	100
All	All	809/819 (99%)	768 (95%)	41 (5%)	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	232/232 (100%)	217 (94%)	15 (6%)	15	45
2	B	95/95 (100%)	89 (94%)	6 (6%)	16	46
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	23
4	D	175/175 (100%)	170 (97%)	5 (3%)	37	68
5	E	212/212 (100%)	199 (94%)	13 (6%)	17	47
All	All	723/723 (100%)	683 (94%)	40 (6%)	19	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	17	ARG
1	A	25	VAL
1	A	73	THR
1	A	74	ASP
1	A	75	ARG
1	A	88	SER
1	A	89	GLU
1	A	110	LEU
1	A	132	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	191	HIS
1	A	248	VAL
1	A	253	GLU
1	A	264	GLU
1	A	273	ARG
2	B	0	MET
2	B	1	ILE
2	B	49	VAL
2	B	53	ASP
2	B	73	THR
2	B	89	GLN
3	C	2	LEU
4	D	4	ASP
4	D	18	SER
4	D	24	THR
4	D	63	THR
4	D	164	ARG
5	E	3	THR
5	E	29	GLU
5	E	31	ASN
5	E	57	GLU
5	E	112	THR
5	E	146	THR
5	E	154	GLU
5	E	156	SER
5	E	191	ARG
5	E	200	GLN
5	E	216	SER
5	E	222	THR
5	E	234	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	70	HIS
1	A	86	ASN
1	A	174	ASN
1	A	180	GLN
1	A	192	HIS
1	A	197	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	13	HIS
2	B	84	HIS
2	B	89	GLN
4	D	7	GLN
4	D	22	ASN
4	D	38	GLN
4	D	58	GLN
4	D	96	ASN
4	D	109	GLN
4	D	122	GLN
5	E	11	HIS
5	E	18	GLN
5	E	31	ASN
5	E	52	ASN
5	E	99	HIS
5	E	101	GLN
5	E	205	HIS
5	E	209	GLN
5	E	211	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
7	EDO	D	201	-	3,3,3	0.63	0	2,2,2	0.63	0
6	MES	A	301	-	12,12,12	0.93	0	15,16,16	0.33	0
8	SO4	E	301	-	4,4,4	0.31	0	6,6,6	0.09	0
8	SO4	E	302	-	4,4,4	0.31	0	6,6,6	0.06	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	201	-	-	1/1/1/1	-
6	MES	A	301	-	-	5/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	MES	C8-C7-N4-C3
6	A	301	MES	C8-C7-N4-C5
6	A	301	MES	C7-C8-S-O2S
6	A	301	MES	C7-C8-S-O3S
7	D	201	EDO	O1-C1-C2-O2
6	A	301	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	201	EDO	4	0
6	A	301	MES	3	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.35	0 100 100	37, 59, 135, 157	0
2	B	100/100 (100%)	-0.39	0 100 100	42, 65, 97, 108	0
3	C	9/9 (100%)	-0.61	0 100 100	40, 45, 59, 61	0
4	D	194/194 (100%)	-0.24	3 (1%) 72 53	35, 59, 111, 125	0
5	E	240/240 (100%)	-0.45	0 100 100	35, 59, 88, 107	0
All	All	819/819 (100%)	-0.36	3 (0%) 88 79	35, 59, 114, 157	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	42	ALA	3.1
4	D	184	CYS	2.3
4	D	194	PRO	2.2

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 oligosaccharides 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
7	EDO	D	201	4/4	0.80	0.24	40,53,55,63	0
8	SO4	E	301	5/5	0.81	0.10	102,113,119,127	0
6	MES	A	301	12/12	0.83	0.14	67,74,117,118	0
8	SO4	E	302	5/5	0.84	0.16	113,119,131,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.