Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 03:50 AM EDT

PDB ID	:	7MLH
Title	:	Crystal structure of human IgE (2F10) in complex with Der p 2.0103
Authors	:	Khatri, K.; Kapingidza, A.B.; Richardson, C.M.; Vailes, L.D.; Wunschmann, S.; Dolamore, C.; Chapman, M.D.; Smith, S.A.; Pomes, A.; Chruszcz, M.
Deposited on	:	2021-04-28
Resolution	:	2.10 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:

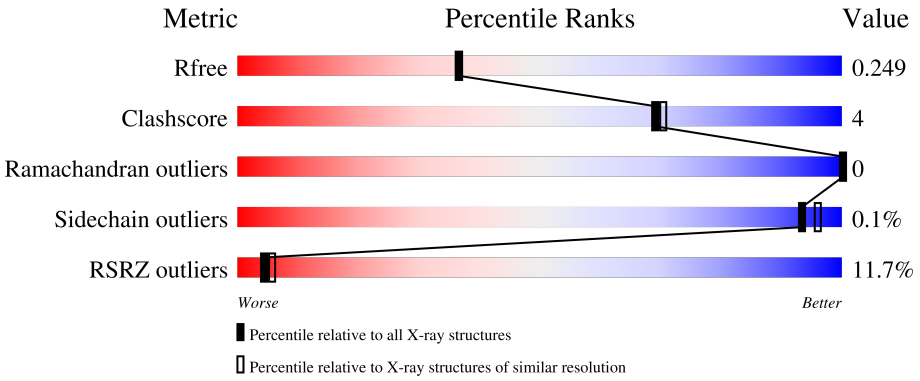
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	212	18% 91% 8%
1	D	212	5% 94% 5%
2	B	129	2% 97%
2	F	129	4% 94% 6%
3	C	228	27% 77% 14% 9%

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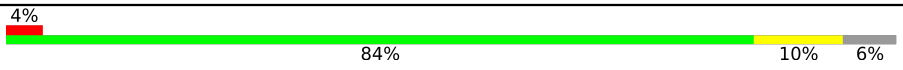
Mol	Chain	Length	Quality of chain
3	E	228	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8935 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 IgE Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1588	995	271	317	5			
1	D	210	Total	C	N	O	S	0	1	0
			1605	1004	274	322	5			

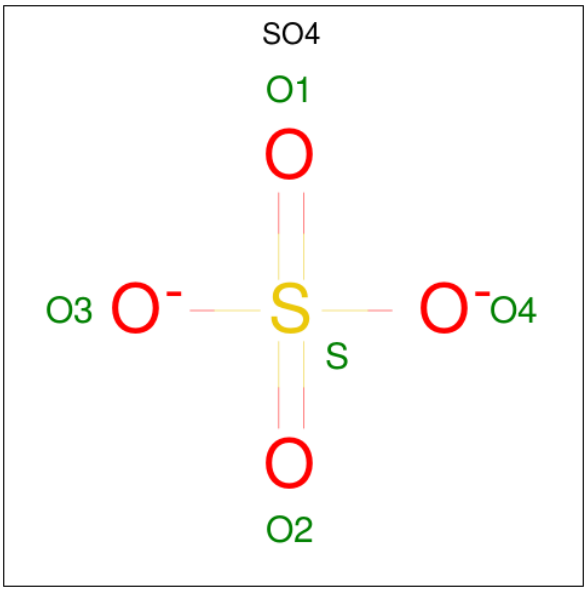
- Molecule 2 is a protein called Der p 2 variant 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			988	623	172	185	8			
2	F	129	Total	C	N	O	S	0	0	0
			988	623	172	185	8			

- Molecule 3 is a protein called IgE Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1519	961	253	299	6			
3	E	215	Total	C	N	O	S	0	0	0
			1587	1001	266	314	6			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	D	2	Total Cl 2 2	0	0

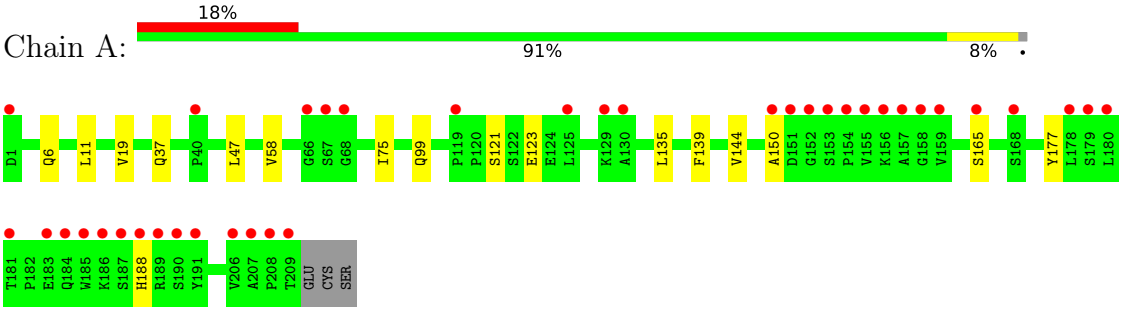
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	83	Total O 83 83	0	0
6	B	99	Total O 99 99	0	0
6	C	42	Total O 42 42	0	0
6	D	152	Total O 152 152	0	0
6	E	140	Total O 140 140	0	0
6	F	66	Total O 66 66	0	0

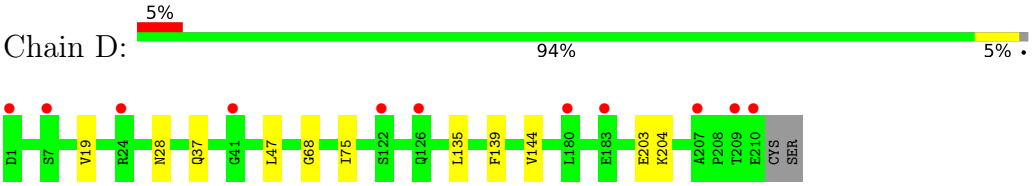
3 Residue-property plots (i)

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.

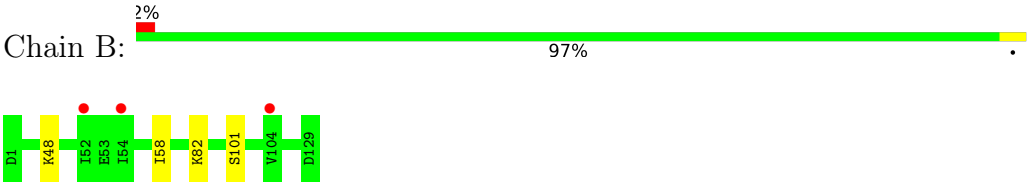
• Molecule 1: IgE Light Chain



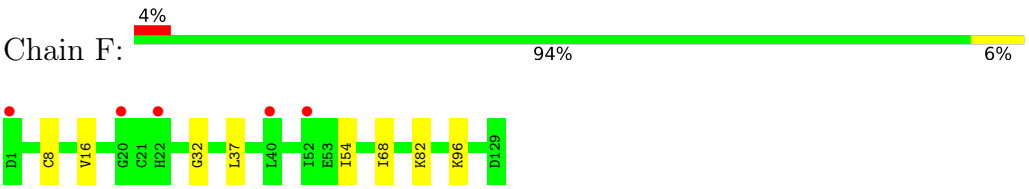
• Molecule 1: IgE Light Chain



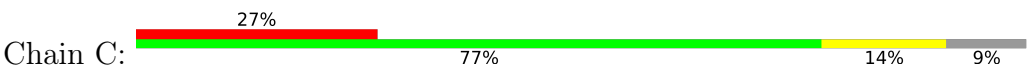
• Molecule 2: Der p 2 variant 3

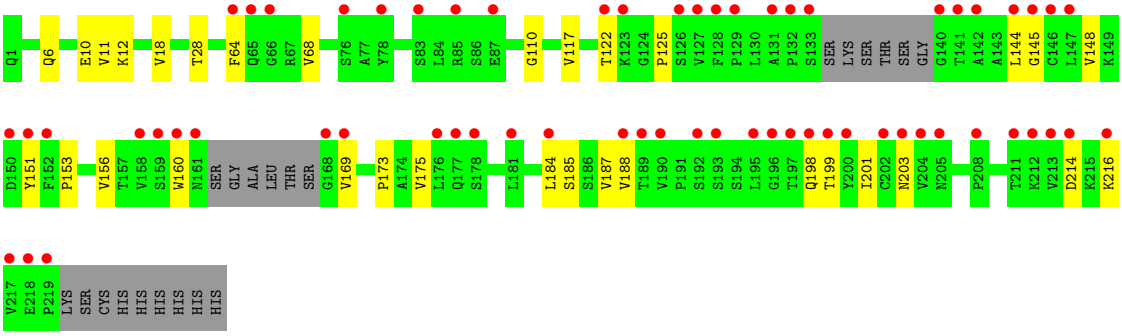


• Molecule 2: Der p 2 variant 3



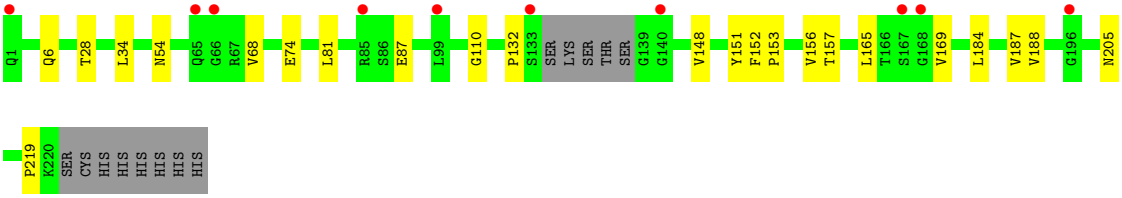
• Molecule 3: IgE Heavy chain





• Molecule 3: IgE Heavy chain

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.78Å 231.46Å 51.79Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	38.61 – 2.10 38.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (38.61-2.10) 96.4 (38.58-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.247 0.217 , 0.249	Depositor DCC
R_{free} test set	3560 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8935	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 8.45% 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: CL, SO4

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	0.66	0/1627	0.83	0/2221
1	D	0.66	1/1644 (0.1%)	0.83	0/2244
2	B	0.63	0/1007	0.79	0/1363
2	F	0.71	0/1007	0.84	0/1363
3	C	0.69	0/1555	0.87	0/2120
3	E	0.72	1/1624 (0.1%)	0.93	0/2210
All	All	0.68	2/8464 (0.0%)	0.85	0/11521

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	GLU	CD-OE2	6.56	1.32	1.25
3	E	87	GLU	CD-OE2	6.28	1.32	1.25

There are no bond angle outliers.

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	1588	0	1545	11	0
1	D	1605	0	1556	7	0
2	B	988	0	998	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	988	0	998	4	1
3	C	1519	0	1462	26	1
3	E	1587	0	1551	16	1
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
4	E	20	0	0	0	0
5	A	1	0	0	0	0
5	D	2	0	0	0	0
6	A	83	0	0	1	0
6	B	99	0	0	1	0
6	C	42	0	0	0	0
6	D	152	0	0	0	0
6	E	140	0	0	0	0
6	F	66	0	0	0	0
All	All	8935	0	8110	61	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 4.

All (61) 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)
3:C:145:GLY:HA2	3:C:160:TRP:CH2	2.25	0.71
3:E:132:PRO:HG2	3:E:219:PRO:HA	1.75	0.66
1:D:135:LEU:HD13	3:E:187:VAL:HG21	1.77	0.66
3:C:169:VAL:HG22	3:C:188:VAL:HG22	1.78	0.65
3:E:151:TYR:CE1	3:E:156:VAL:HG23	2.31	0.65
3:E:165:LEU:HD21	3:E:188:VAL:HG11	1.77	0.65
3:C:151:TYR:CE1	3:C:156:VAL:HG23	2.32	0.64
2:F:54:ILE:HD12	2:F:68:ILE:HG21	1.84	0.60
3:E:148:VAL:HG11	3:E:156:VAL:HG11	1.83	0.60
3:E:169:VAL:HG22	3:E:188:VAL:HG22	1.84	0.59
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.85	0.58
3:C:184:LEU:HD12	3:C:185:SER:N	2.19	0.57
3:E:34:LEU:C	3:E:34:LEU:HD13	2.27	0.54
3:C:184:LEU:HD12	3:C:184:LEU:C	2.28	0.54
1:A:165:SER:OG	3:C:173:PRO:HG2	2.09	0.53
3:C:125:PRO:HB3	3:C:151:TYR:HB3	1.89	0.53
3:E:54:ASN:ND2	3:E:74:GLU:HG2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:VAL:HG11	3:C:156:VAL:HG11	1.92	0.52
3:C:144:LEU:C	3:C:144:LEU:HD12	2.30	0.52
2:B:58:ILE:HG23	2:B:101:SER:HB2	1.93	0.51
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.92	0.51
1:D:139:PHE:CE1	1:D:144:VAL:HG13	2.46	0.50
3:C:64:PHE:HB3	3:C:68:VAL:CG2	2.42	0.50
2:F:16:VAL:HG13	2:F:37:LEU:HD11	1.94	0.49
3:C:198:GLN:HG3	3:C:199:THR:N	2.29	0.48
3:C:145:GLY:HA2	3:C:160:TRP:HH2	1.75	0.48
3:C:201:ILE:HD13	3:C:216:LYS:HA	1.96	0.47
1:A:177:TYR:CD2	3:C:175:VAL:HG11	2.49	0.47
1:A:135:LEU:HD12	3:C:187:VAL:HG21	1.96	0.46
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.98	0.46
3:E:6:GLN:OE1	3:E:110:GLY:HA3	2.15	0.45
3:C:151:TYR:OH	3:C:184:LEU:HD23	2.17	0.45
2:F:16:VAL:CG1	2:F:37:LEU:HD11	2.47	0.45
1:A:19:VAL:HG22	1:A:75:ILE:HB	1.97	0.45
2:B:48:LYS:NZ	6:B:301:HOH:O	2.29	0.45
1:D:28:ASN:OD1	1:D:68:GLY:HA2	2.16	0.45
1:A:121:SER:HB2	1:A:123:GLU:OE1	2.17	0.45
3:C:11:VAL:CG2	3:C:153:PRO:HD3	2.46	0.45
1:A:11:LEU:HD21	1:A:19:VAL:HB	1.98	0.44
3:C:10:GLU:OE2	3:C:18:VAL:HG23	2.17	0.44
3:C:6:GLN:OE1	3:C:110:GLY:HA3	2.18	0.44
3:C:122:THR:HG22	3:C:153:PRO:HD3	1.99	0.44
1:D:135:LEU:HD13	3:E:187:VAL:CG2	2.45	0.43
3:E:68:VAL:HG22	3:E:81:LEU:HD13	2.00	0.43
3:C:145:GLY:HA2	3:C:160:TRP:CZ2	2.54	0.43
3:E:54:ASN:HD22	3:E:74:GLU:HG2	1.83	0.42
3:C:151:TYR:CE1	3:C:156:VAL:CG2	3.00	0.42
1:A:150:ALA:HB1	1:A:188:HIS:CD2	2.53	0.42
3:E:151:TYR:CE1	3:E:156:VAL:CG2	3.02	0.42
1:A:139:PHE:CE2	1:A:144:VAL:HG13	2.55	0.42
3:C:12:LYS:O	3:C:117:VAL:HA	2.19	0.42
3:C:64:PHE:HB3	3:C:68:VAL:HG21	2.02	0.42
1:A:6:GLN:O	1:A:99:GLN:NE2	2.47	0.41
6:A:410:HOH:O	1:D:204:LYS:HE3	2.21	0.41
3:C:203:ASN:HA	3:C:214:ASP:OD1	2.21	0.41
1:D:19:VAL:HG22	1:D:75:ILE:HB	2.02	0.41
2:F:32:GLY:HA3	2:F:96:LYS:HG2	2.03	0.41
3:C:148:VAL:HB	3:C:184:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:184:LEU:C	3:E:184:LEU:HD12	2.42	0.40
3:E:152:PHE:HA	3:E:153:PRO:HA	1.90	0.40
3:E:157:THR:OG1	3:E:205:ASN:HB3	2.22	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)
3:C:28:THR:OG1	2:F:82:LYS:NZ[1_556]	1.86	0.34
2:B:82:LYS:NZ	3:E:28:THR:OG1[1_554]	2.09	0.11

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	207/212 (98%)	203 (98%)	4 (2%)	0	100	100
1	D	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
2	B	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
2	F	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
3	C	201/228 (88%)	196 (98%)	5 (2%)	0	100	100
3	E	211/228 (92%)	207 (98%)	4 (2%)	0	100	100
All	All	1082/1138 (95%)	1060 (98%)	22 (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	178/183 (97%)	178 (100%)	0	100 100
1	D	180/183 (98%)	180 (100%)	0	100 100
2	B	110/110 (100%)	110 (100%)	0	100 100
2	F	110/110 (100%)	109 (99%)	1 (1%)	78 84
3	C	166/190 (87%)	166 (100%)	0	100 100
3	E	176/190 (93%)	176 (100%)	0	100 100
All	All	920/966 (95%)	919 (100%)	1 (0%)	93 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	8	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	197	HIS

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)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	303	-	4,4,4	0.47	0	6,6,6	0.05	0
4	SO4	A	302	-	4,4,4	0.43	0	6,6,6	0.05	0
4	SO4	C	301	-	4,4,4	0.48	0	6,6,6	0.06	0
4	SO4	A	301	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	B	202	-	4,4,4	0.43	0	6,6,6	0.05	0
4	SO4	D	301	-	4,4,4	0.49	0	6,6,6	0.06	0
4	SO4	B	203	-	4,4,4	0.51	0	6,6,6	0.06	0
4	SO4	E	304	-	4,4,4	0.48	0	6,6,6	0.04	0
4	SO4	C	302	-	4,4,4	0.45	0	6,6,6	0.05	0
4	SO4	D	303	-	4,4,4	0.49	0	6,6,6	0.06	0
4	SO4	E	301	-	4,4,4	0.51	0	6,6,6	0.07	0
4	SO4	E	303	-	4,4,4	0.48	0	6,6,6	0.07	0
4	SO4	D	302	-	4,4,4	0.46	0	6,6,6	0.04	0
4	SO4	E	302	-	4,4,4	0.53	0	6,6,6	0.05	0
4	SO4	B	201	-	4,4,4	0.43	0	6,6,6	0.05	0

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.

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, 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	209/212 (98%)	1.15	38 (18%) 1 1	28, 45, 95, 107	0
1	D	210/212 (99%)	0.55	11 (5%) 27 32	22, 33, 51, 90	0
2	B	129/129 (100%)	0.59	3 (2%) 60 65	24, 36, 46, 53	0
2	F	129/129 (100%)	0.54	5 (3%) 39 45	32, 44, 58, 64	0
3	C	207/228 (90%)	1.67	62 (29%) 0 0	32, 59, 113, 141	0
3	E	215/228 (94%)	0.59	10 (4%) 31 37	23, 34, 59, 70	0
All	All	1099/1138 (96%)	0.89	129 (11%) 4 6	22, 40, 90, 141	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	195	LEU	11.1
3	C	196	GLY	9.6
1	D	209	THR	9.5
3	E	133	SER	8.5
1	A	180	LEU	8.2
3	C	213	VAL	7.9
1	A	156	LYS	7.9
3	C	202	CYS	7.2
3	C	169	VAL	7.1
1	A	157	ALA	7.1
3	C	160	TRP	7.0
3	C	64	PHE	6.9
3	C	217	VAL	6.5
1	A	191	TYR	6.2
1	A	67	SER	5.7
3	C	193	SER	5.7
1	A	207	ALA	5.4
3	C	128	PHE	5.3
3	C	65	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
3	C	214	ASP	5.0
1	A	185	TRP	4.9
3	C	219	PRO	4.9
3	C	211	THR	4.9
3	C	144	LEU	4.9
1	A	187	SER	4.7
1	A	151	ASP	4.5
3	C	216	LYS	4.5
3	C	168	GLY	4.3
3	C	197	THR	4.3
3	C	199	THR	4.3
3	C	133	SER	4.2
1	A	189	ARG	4.1
3	C	140	GLY	4.0
3	C	150	ASP	4.0
3	C	204	VAL	4.0
1	A	129	LYS	3.9
3	C	126	SER	3.9
3	C	122	THR	3.8
3	C	131	ALA	3.7
1	A	208	PRO	3.7
3	C	132	PRO	3.6
1	A	66	GLY	3.6
1	A	152	GLY	3.6
1	A	68	GLY	3.6
3	E	66	GLY	3.6
3	C	200	TYR	3.5
1	A	153	SER	3.5
1	A	125	LEU	3.5
1	A	183	GLU	3.5
1	A	150	ALA	3.5
3	C	85	ARG	3.4
3	C	158	VAL	3.4
1	D	210	GLU	3.3
3	C	151	TYR	3.3
3	E	140	GLY	3.3
3	C	127	VAL	3.2
3	C	76	SER	3.2
3	C	177	GLN	3.1
3	C	176	LEU	3.1
1	A	155	VAL	3.0
3	E	65	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	3.0
3	C	141	THR	2.9
2	F	20	GLY	2.9
3	C	205	ASN	2.9
3	C	178	SER	2.9
3	C	192	SER	2.9
1	A	184	GLN	2.8
3	C	142	ALA	2.7
2	F	22	HIS	2.7
3	C	190	VAL	2.6
1	A	168	SER	2.6
3	C	66	GLY	2.6
3	C	146	CYS	2.6
3	C	78	TYR	2.6
3	C	184	LEU	2.6
3	E	167	SER	2.5
3	C	145	GLY	2.5
1	A	159	VAL	2.5
1	A	165	SER	2.5
1	A	190	SER	2.5
3	C	123	LYS	2.5
3	C	129	PRO	2.4
1	A	40	PRO	2.4
1	D	1	ASP	2.4
3	E	1	GLN	2.4
1	A	186	LYS	2.4
3	C	159	SER	2.4
1	A	130	ALA	2.4
3	C	203	ASN	2.3
1	D	41	GLY	2.3
3	E	168	GLY	2.3
1	A	181	THR	2.3
1	D	122	SER	2.3
3	C	218	GLU	2.3
3	C	161	ASN	2.3
3	E	85	ARG	2.3
2	B	54	ILE	2.3
3	C	189	THR	2.2
3	C	208	PRO	2.2
2	F	52	ILE	2.2
2	F	40	LEU	2.2
1	D	126	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	212	LYS	2.2
3	E	99	LEU	2.2
1	A	179	SER	2.2
2	B	104	VAL	2.2
1	A	209	THR	2.2
3	C	188	VAL	2.1
2	F	1	ASP	2.1
3	E	196	GLY	2.1
1	D	183	GLU	2.1
1	A	188	HIS	2.1
3	C	152	PHE	2.1
1	A	154	PRO	2.1
1	A	158	GLY	2.1
3	C	181	LEU	2.1
1	A	206	VAL	2.1
3	C	87	GLU	2.1
3	C	198	GLN	2.1
1	A	1	ASP	2.1
1	D	7	SER	2.0
1	D	24	ARG	2.0
1	A	119	PRO	2.0
1	D	180	LEU	2.0
3	C	83	SER	2.0
1	D	207	ALA	2.0
2	B	52	ILE	2.0
3	C	147	LEU	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
4	SO4	B	202	5/5	0.57	0.39	55,74,84,84	0
4	SO4	B	201	5/5	0.74	0.29	78,84,94,96	0
4	SO4	D	301	5/5	0.77	0.30	66,67,79,82	0
4	SO4	A	302	5/5	0.83	0.28	103,107,110,111	0
4	SO4	E	303	5/5	0.83	0.21	57,65,75,82	0
4	SO4	A	301	5/5	0.87	0.25	72,79,86,87	0
4	SO4	C	302	5/5	0.87	0.62	32,32,32,32	0
4	SO4	D	302	5/5	0.89	0.24	62,68,78,83	0
4	SO4	A	303	5/5	0.90	0.24	75,78,83,83	0
4	SO4	E	304	5/5	0.93	0.51	32,32,32,32	0
4	SO4	E	301	5/5	0.95	0.25	59,62,69,73	0
4	SO4	C	301	5/5	0.95	0.31	77,78,79,85	0
4	SO4	D	303	5/5	0.95	0.16	62,62,65,66	0
4	SO4	E	302	5/5	0.96	0.17	43,44,47,55	0
4	SO4	B	203	5/5	0.97	0.11	52,56,63,66	0
5	CL	D	304	1/1	0.97	0.11	32,32,32,32	0
5	CL	A	304	1/1	0.99	0.07	32,32,32,32	0
5	CL	D	305	1/1	0.99	0.13	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.