Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:04 pm BST

PDB ID	:	6HF1
Title	:	Mutant oxidoreductase fragment of mouse QSOX1 in complex with an antibody Fab
Authors	:	Grossman-Haham, I.; Fass, D.
Deposited on	:	2018-08-21
Resolution	:	1.94 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 following versions of software and data (see references ⓘ) were used in the production of this report:

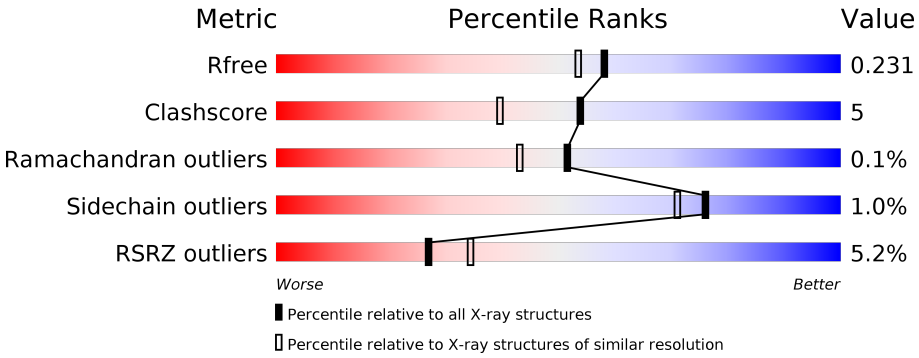
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 on 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	238	6% 85% 15%
1	D	238	8% 85% 15%
2	C	215	4% 88% 9% .
3	B	212	9% 87% 12%
3	E	212	% 92% 8%
4	F	216	% 87% 10% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10954 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 Sulfhydryl oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	2	0
			1854	1179	318	350	7			
1	D	238	Total	C	N	O	S	0	0	0
			1847	1173	318	349	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ALA	HIS	engineered mutation	UNP Q8BND5
A	122	THR	PRO	engineered mutation	UNP Q8BND5
D	75	ALA	HIS	engineered mutation	UNP Q8BND5
D	122	THR	PRO	engineered mutation	UNP Q8BND5

- Molecule 2 is a protein called Fab 316 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	2	0
			1603	1024	261	313	5			

- Molecule 3 is a protein called Fab 316 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	211	Total	C	N	O	S	0	1	0
			1616	1015	267	327	7			
3	E	212	Total	C	N	O	S	0	2	0
			1627	1022	269	329	7			

- Molecule 4 is a protein called Fab 316 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	210	Total	C	N	O	S	0	1	0
			1603	1024	261	313	5			

- Molecule 5 is water.

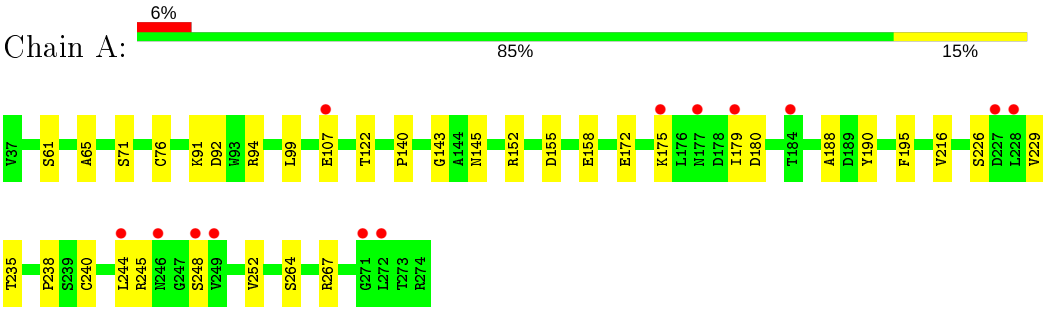
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0
5	C	133	Total O 133 133	0	0
5	B	163	Total O 163 163	0	0
5	D	101	Total O 101 101	0	0
5	F	155	Total O 155 155	0	0
5	E	126	Total O 126 126	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

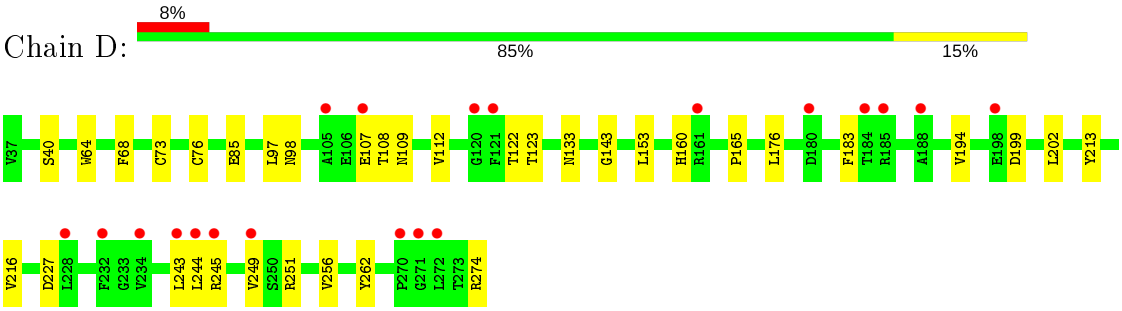
- Molecule 1: Sulfhydryl oxidase 1

Chain A:



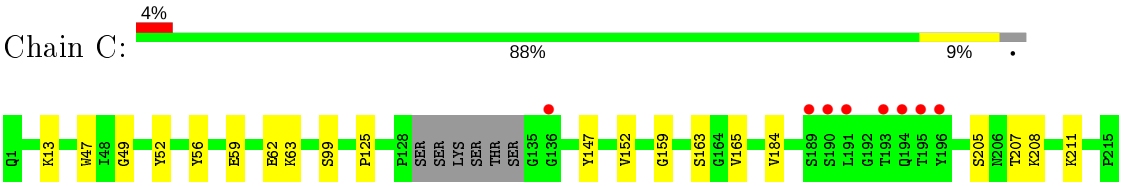
- Molecule 1: Sulfhydryl oxidase 1

Chain D:



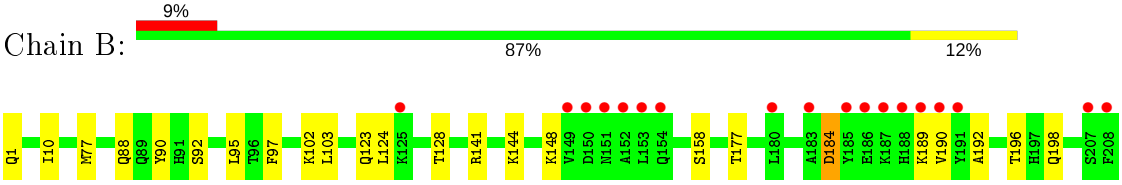
- Molecule 2: Fab 316 heavy chain

Chain C:



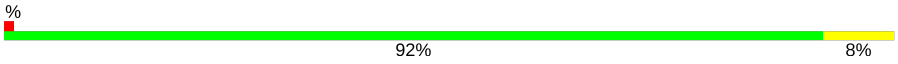
- Molecule 3: Fab 316 light chain

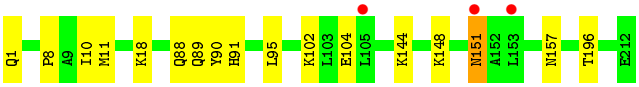
Chain B:



- Molecule 3: Fab 316 light chain

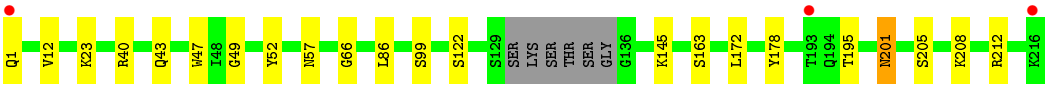
Chain E:





- Molecule 4: Fab 316 heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.54Å 112.72Å 193.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 1.94 48.89 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.89-1.94) 97.6 (48.89-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.194 , 0.231 0.194 , 0.231	Depositor DCC
R_{free} test set	5215 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10954	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

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	0.40	0/1904	0.58	0/2598
1	D	0.38	0/1891	0.54	0/2580
2	C	0.41	0/1654	0.58	0/2258
3	B	0.38	0/1659	0.56	0/2255
3	E	0.42	0/1673	0.59	0/2274
4	F	0.40	0/1651	0.58	0/2255
All	All	0.40	0/10432	0.57	0/14220

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
2	C	0	1
4	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	99	SER	Peptide
4	F	99	SER	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	1854	0	1815	29	1
1	D	1847	0	1801	24	0
2	C	1603	0	1559	13	2
3	B	1616	0	1564	23	0
3	E	1627	0	1574	11	0
4	F	1603	0	1552	15	0
5	A	126	0	0	10	1
5	B	163	0	0	4	0
5	C	133	0	0	3	0
5	D	101	0	0	2	0
5	E	126	0	0	4	0
5	F	155	0	0	5	0
All	All	10954	0	9865	106	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 5.

All (106) 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:B:10:ILE:HD13	3:B:102:LYS:HB3	1.34	1.06
3:B:144:LYS:NZ	5:B:301:HOH:O	1.92	1.02
1:A:61:SER:O	5:A:302:HOH:O	1.83	0.95
3:B:1:GLN:N	3:B:1:GLN:OE1	2.09	0.86
3:B:10:ILE:HD12	3:B:102:LYS:O	1.80	0.82
1:A:158:GLU:OE2	5:A:303:HOH:O	1.99	0.81
3:B:10:ILE:CD1	3:B:102:LYS:HB3	2.15	0.75
3:B:10:ILE:HD13	3:B:102:LYS:CB	2.13	0.75
1:D:107:GLU:N	1:D:107:GLU:OE1	2.20	0.75
1:A:179:ILE:HB	5:A:311:HOH:O	1.87	0.74
4:F:43:GLN:OE1	5:F:301:HOH:O	2.06	0.73
1:A:172:GLU:OE2	5:A:304:HOH:O	2.08	0.71
1:A:71:SER:O	5:A:305:HOH:O	2.09	0.69
3:E:18:LYS:NZ	5:E:301:HOH:O	2.25	0.69
1:D:243:LEU:HG	1:D:249:VAL:HG22	1.74	0.69
1:A:180:ASP:N	5:A:311:HOH:O	2.25	0.68
1:D:85:GLU:OE2	5:D:301:HOH:O	2.11	0.68
4:F:23:LYS:HD2	5:F:336:HOH:O	1.93	0.68
2:C:159:GLY:O	5:C:301:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:O	5:A:306:HOH:O	2.14	0.66
3:E:91:HIS:ND1	5:E:303:HOH:O	2.28	0.66
1:A:238:PRO:O	5:A:307:HOH:O	2.14	0.65
3:E:148:LYS:HB3	3:E:151:ASN:HA	1.80	0.63
1:D:213:TYR:OH	1:D:274:ARG:NH1	2.27	0.62
2:C:62:GLU:OE2	5:C:302:HOH:O	2.16	0.62
1:D:183:PHE:O	1:D:245:ARG:NH2	2.33	0.61
1:A:122:THR:OG1	5:A:308:HOH:O	2.16	0.60
1:D:68:PHE:O	1:D:122:THR:HA	2.02	0.60
3:E:1:GLN:N	3:E:1:GLN:OE1	2.30	0.60
4:F:40[A]:ARG:NE	5:F:301:HOH:O	2.29	0.60
1:A:91:LYS:HD2	1:A:94:ARG:HD2	1.85	0.59
3:B:1:GLN:CD	3:B:1:GLN:H1	2.02	0.58
1:A:91:LYS:HE3	1:A:94:ARG:HH11	1.68	0.57
1:D:216:VAL:O	5:D:302:HOH:O	2.18	0.57
1:A:65:ALA:HB3	1:A:99:LEU:HD22	1.87	0.57
1:D:107:GLU:HG2	1:D:108:THR:N	2.18	0.56
1:A:152[B]:ARG:NH1	1:A:155:ASP:OD2	2.38	0.56
2:C:13:LYS:HE3	1:D:256:VAL:HG13	1.87	0.56
2:C:125:PRO:HD3	2:C:211:LYS:HE2	1.88	0.55
1:A:92:ASP:OD2	1:A:267:ARG:NH2	2.40	0.55
1:A:76:CYS:SG	1:A:122:THR:HB	2.47	0.54
1:A:190:TYR:HB2	1:A:216:VAL:HG22	1.88	0.54
3:B:148:LYS:HB2	3:B:192:ALA:HB3	1.88	0.54
4:F:66:GLY:N	5:F:302:HOH:O	2.09	0.53
3:B:141:ARG:NH1	5:B:311:HOH:O	2.41	0.53
3:E:10:ILE:HD11	3:E:104:GLU:OE1	2.09	0.53
1:A:244:LEU:HD23	1:A:248:SER:OG	2.08	0.53
1:A:188:ALA:O	1:A:245:ARG:NH1	2.43	0.52
3:E:157:ASN:HB2	5:E:361:HOH:O	2.08	0.52
1:A:226:SER:HA	1:A:229:VAL:HB	1.92	0.51
3:B:198:GLN:NE2	5:B:302:HOH:O	2.19	0.51
2:C:63:LYS:NZ	5:C:304:HOH:O	2.32	0.51
1:A:195:PHE:O	1:A:238:PRO:HA	2.12	0.49
1:D:97:LEU:HD21	1:D:153:LEU:HD13	1.95	0.49
1:D:176:LEU:HD22	1:D:227:ASP:HB3	1.95	0.49
3:E:8:PRO:HG2	3:E:11:MET:HB3	1.95	0.48
1:D:107:GLU:HG2	1:D:108:THR:H	1.78	0.48
1:D:109:ASN:O	1:D:112:VAL:HG12	2.13	0.47
1:A:143:GLY:HA3	2:C:52:TYR:CD2	2.49	0.47
1:A:145:ASN:HB2	2:C:59:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:ILE:HD13	3:E:102:LYS:HB3	1.96	0.47
1:D:202:LEU:HD21	1:D:262:TYR:CE2	2.50	0.47
3:E:90:TYR:HA	3:E:95:LEU:HD22	1.97	0.46
4:F:12:VAL:HG21	4:F:86:LEU:HD13	1.97	0.46
4:F:145:LYS:HE2	5:E:304:HOH:O	2.15	0.46
4:F:195:THR:HG23	4:F:212:ARG:HD2	1.98	0.46
1:D:160:HIS:CD2	1:D:165:PRO:HD3	2.51	0.46
3:B:184:ASP:N	3:B:184:ASP:OD1	2.49	0.46
2:C:147:TYR:CE2	2:C:152:VAL:HG13	2.52	0.45
1:A:143:GLY:HA3	2:C:52:TYR:CG	2.51	0.45
1:A:264[B]:SER:HB2	4:F:205:SER:HB2	1.98	0.45
4:F:122:SER:OG	5:F:303:HOH:O	2.21	0.45
3:B:210:ARG:HA	3:B:211:GLY:HA2	1.63	0.45
1:A:264[A]:SER:HB3	4:F:205:SER:HB2	1.99	0.44
3:B:10:ILE:HD13	3:B:102:LYS:CG	2.46	0.44
2:C:13:LYS:HE3	1:D:256:VAL:CG1	2.48	0.44
1:D:122:THR:O	1:D:123:THR:OG1	2.28	0.44
3:B:92:SER:HB3	5:B:400:HOH:O	2.17	0.44
3:B:144:LYS:HB3	3:B:196:THR:HB	1.99	0.44
1:A:240:CYS:HB3	1:A:252:VAL:HB	2.00	0.43
1:A:152[B]:ARG:HA	1:A:152[B]:ARG:HD3	1.69	0.43
3:B:190:VAL:HG22	3:B:209:ASN:OD1	2.19	0.43
1:D:143:GLY:HA3	4:F:52:TYR:CG	2.53	0.43
3:B:124:LEU:HD23	3:B:124:LEU:HA	1.84	0.43
4:F:172:LEU:HD13	4:F:178:TYR:CZ	2.54	0.43
1:A:140:PRO:O	1:A:152[A]:ARG:NH1	2.52	0.42
3:B:88:GLN:HG3	3:B:97:PHE:CE2	2.54	0.42
3:E:88:GLN:NE2	3:E:89:GLN:O	2.53	0.42
1:D:73:CYS:HB3	1:D:76:CYS:SG	2.59	0.42
3:B:90:TYR:HA	3:B:95:LEU:HD22	2.01	0.42
1:A:248:SER:HA	5:A:313:HOH:O	2.20	0.42
3:B:77:MET:SD	3:B:103:LEU:HD21	2.59	0.42
2:C:165:VAL:HG22	2:C:184:VAL:HB	2.02	0.42
3:B:189:LYS:HG2	3:B:190:VAL:HG23	2.02	0.42
1:D:194:VAL:HG11	1:D:202:LEU:HD23	2.02	0.41
1:D:143:GLY:HA3	4:F:52:TYR:CD2	2.55	0.41
3:B:158:SER:HA	3:B:177:THR:O	2.20	0.41
1:D:64:TRP:CZ3	1:D:98:ASN:HB3	2.55	0.41
3:B:123:GLN:HG2	3:B:128:THR:O	2.20	0.41
1:D:244:LEU:HD12	1:D:244:LEU:HA	1.70	0.41
4:F:47:TRP:CZ2	4:F:49:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:SER:O	2:C:207:THR:HG23	2.21	0.41
3:E:144:LYS:HB3	3:E:196:THR:HB	2.02	0.41
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.56	0.41
1:D:199:ASP:OD1	1:D:199:ASP:N	2.54	0.40
4:F:201:ASN:ND2	4:F:208:LYS:HG2	2.36	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:C:56:TYR:OH	5:A:301:HOH:O[4_555]	1.93	0.27
1:A:107:GLU:OE1	2:C:56:TYR:OH[4_455]	2.14	0.06

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	238/238 (100%)	231 (97%)	7 (3%)	0	100	100
1	D	236/238 (99%)	230 (98%)	6 (2%)	0	100	100
2	C	207/215 (96%)	202 (98%)	5 (2%)	0	100	100
3	B	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
3	E	212/212 (100%)	204 (96%)	7 (3%)	1 (0%)	29	17
4	F	207/216 (96%)	203 (98%)	4 (2%)	0	100	100
All	All	1310/1331 (98%)	1274 (97%)	35 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	151	ASN

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	201/201 (100%)	200 (100%)	1 (0%)	88	88
1	D	199/201 (99%)	196 (98%)	3 (2%)	65	56
2	C	179/183 (98%)	177 (99%)	2 (1%)	73	67
3	B	184/184 (100%)	183 (100%)	1 (0%)	88	88
3	E	185/184 (100%)	185 (100%)	0	100	100
4	F	178/184 (97%)	174 (98%)	4 (2%)	52	39
All	All	1126/1137 (99%)	1115 (99%)	11 (1%)	76	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
2	C	163	SER
2	C	208	LYS
3	B	184	ASP
1	D	40	SER
1	D	133	ASN
1	D	251	ARG
4	F	1	GLN
4	F	57	ASN
4	F	163	SER
4	F	201	ASN

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

Mol	Chain	Res	Type
2	C	5	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	238/238 (100%)	0.70	15 (6%) 20 26	26, 42, 67, 74	0
1	D	238/238 (100%)	0.55	20 (8%) 11 16	31, 44, 71, 79	0
2	C	209/215 (97%)	0.44	8 (3%) 40 48	23, 38, 67, 83	0
3	B	211/212 (99%)	0.49	20 (9%) 8 12	24, 37, 65, 72	0
3	E	212/212 (100%)	0.14	3 (1%) 75 80	30, 41, 54, 70	0
4	F	210/216 (97%)	0.23	3 (1%) 75 80	27, 36, 52, 65	0
All	All	1318/1331 (99%)	0.43	69 (5%) 27 34	23, 39, 66, 83	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	193	THR	5.4
1	D	184	THR	4.5
3	B	183	ALA	4.5
3	B	190	VAL	4.4
3	B	149	VAL	4.2
1	D	232	PHE	4.1
1	D	120	GLY	4.1
3	B	208	PHE	3.9
1	A	248	SER	3.9
3	B	210	ARG	3.7
1	A	244	LEU	3.7
3	B	151	ASN	3.6
4	F	193	THR	3.6
3	B	180	LEU	3.5
3	B	150	ASP	3.4
4	F	1	GLN	3.4
2	C	196	TYR	3.4
1	D	180	ASP	3.4
2	C	136	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	184	THR	3.2
3	E	151	ASN	3.2
1	A	179	ILE	3.0
1	A	271	GLY	3.0
1	D	185	ARG	3.0
2	C	189	SER	3.0
1	A	175	LYS	3.0
3	B	186	GLU	2.9
1	D	244	LEU	2.9
3	B	209	ASN	2.9
1	D	249	VAL	2.9
1	A	272	LEU	2.8
1	D	198	GLU	2.8
3	B	185	TYR	2.8
3	B	187	LYS	2.7
3	B	153	LEU	2.7
1	A	232	PHE	2.7
1	A	249	VAL	2.7
3	E	153	LEU	2.7
1	A	227	ASP	2.6
1	D	121	PHE	2.6
1	A	234	VAL	2.6
3	B	188	HIS	2.6
1	A	107	GLU	2.6
1	D	271	GLY	2.6
3	B	191	TYR	2.6
2	C	195	THR	2.6
1	D	105	ALA	2.5
1	D	243	LEU	2.5
1	A	246	ASN	2.5
1	D	161	ARG	2.5
3	B	207	SER	2.5
1	D	270	PRO	2.5
3	B	154	GLN	2.5
3	B	189	LYS	2.4
1	A	228	LEU	2.4
1	D	107	GLU	2.4
1	D	272	LEU	2.4
1	D	234	VAL	2.3
1	A	177	ASN	2.2
1	D	245	ARG	2.2
2	C	191	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	105	LEU	2.2
3	B	125	LYS	2.2
2	C	190	SER	2.2
2	C	194	GLN	2.1
4	F	216	LYS	2.1
1	D	188	ALA	2.1
3	B	152	ALA	2.0
1	D	228	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.