



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 04:04 pm GMT

PDB ID : 6Z7Z
Title : Porcine insulin in complex with the analytical antibody OXI-005 Fab
Authors : Johansson, E.
Deposited on : 2020-06-02
Resolution : 2.40 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 : 2.16
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) : 2.16

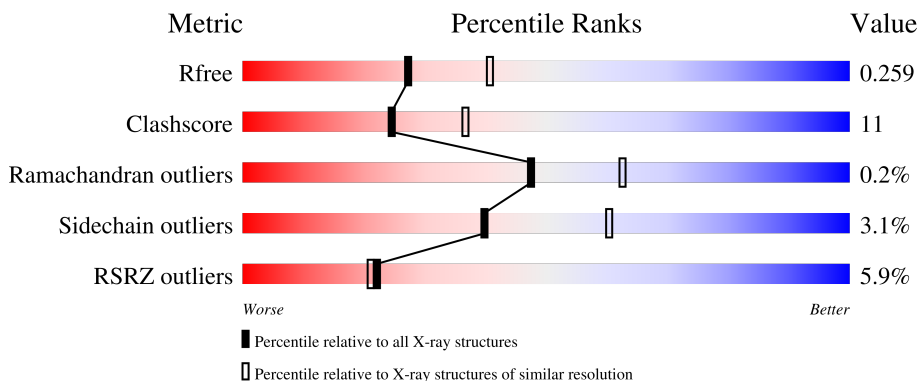
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	213	<div style="display: flex; align-items: center;"> <div style="width: 19%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">19% 73% 25% ..</p>
1	C	213	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">75% 23% ..</p>
2	B	220	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">4% 75% 20% . 5%</p>
2	D	220	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="text-align: center;">2% 77% 21% ..</p>
3	E	21	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">67% 29% 5%</p>

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Mol	Chain	Length	Quality of chain
3	G	21	 90% 10%
4	F	30	 7% 80% 17%
4	H	30	 80% 13% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7705 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 OXI-005 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1638	C 1023	N 278	O 331	S 6	0	0	0
1	C	211	Total 1638	C 1023	N 278	O 331	S 6	0	0	0

- Molecule 2 is a protein called OXI-005 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	210	Total 1605	C 1024	N 258	O 316	S 7	0	0	0
2	D	218	Total 1666	C 1057	N 271	O 330	S 8	0	1	0

- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
3	G	21	Total 163	C 99	N 25	O 35	S 4	0	0	0

- Molecule 4 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	29	Total 229	C 148	N 39	O 40	S 2	0	0	0
4	H	28	Total 222	C 143	N 38	O 39	S 2	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

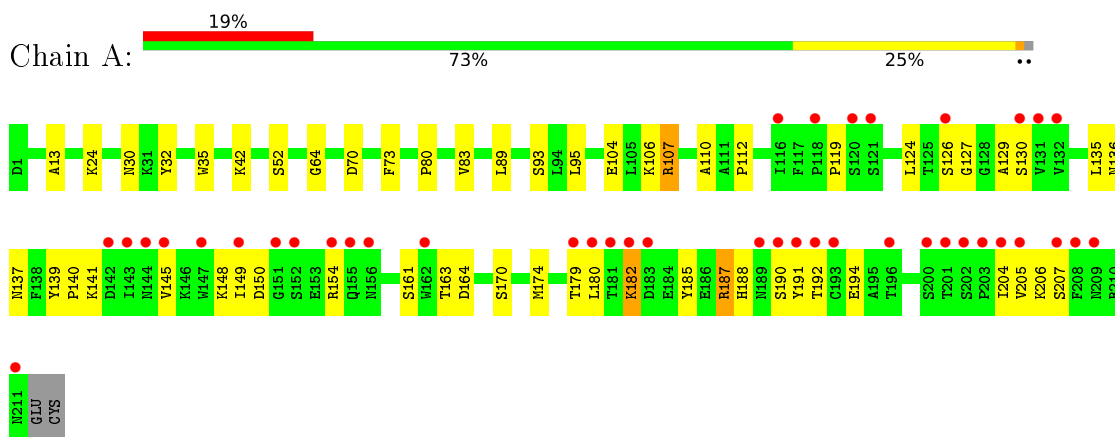
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	88	Total O 88 88	0	0
6	C	77	Total O 77 77	0	0
6	D	115	Total O 115 115	0	0
6	E	8	Total O 8 8	0	0
6	F	10	Total O 10 10	0	0
6	G	15	Total O 15 15	0	0
6	H	5	Total O 5 5	0	0

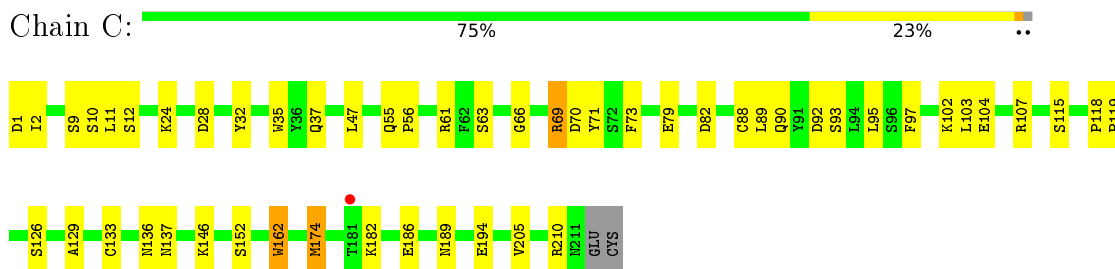
3 Residue-property plots [i](#)

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.

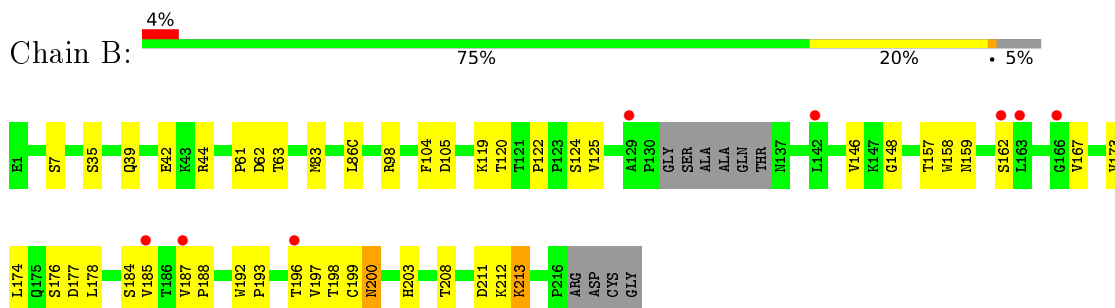
- Molecule 1: OXI-005 Fab Light chain




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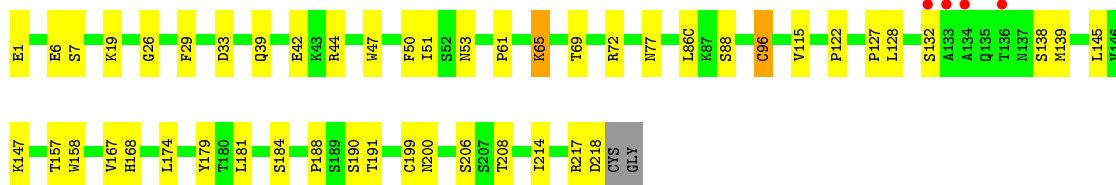


- Molecule 2: OXI-005 Fab Heavy chain



- Molecule 2: OXI-005 Fab Heavy chain

Chain D:  77% 21% 2% ..




• Molecule 3: Insulin

Chain E:  67% 29% 5%




• Molecule 3: Insulin

Chain G:  90% 10%




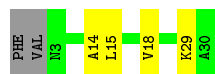
• Molecule 4: Insulin

Chain F:  80% 17% 7%



• Molecule 4: Insulin

Chain H:  80% 13% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.67Å 171.55Å 83.17Å 90.00° 135.89° 90.00°	Depositor
Resolution (Å)	47.99 – 2.40 47.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.99-2.40) 96.7 (47.99-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.39Å)	Xtrriage
Refinement program	PHENIX dev_3714	Depositor
R, R_{free}	0.210 , 0.259 0.210 , 0.259	Depositor DCC
R_{free} test set	1476 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.2	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	0.93	EDS
Total number of atoms	7705	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: MG

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	0.42	0/1676	0.66	0/2274
1	C	0.44	0/1676	0.66	1/2274 (0.0%)
2	B	0.45	0/1648	0.65	1/2252 (0.0%)
2	D	0.51	1/1710 (0.1%)	0.69	2/2337 (0.1%)
3	E	0.47	0/164	0.69	0/220
3	G	0.67	0/164	0.65	0/220
4	F	0.51	0/235	0.56	0/316
4	H	0.39	0/228	0.60	0/306
All	All	0.46	1/7501 (0.0%)	0.66	4/10199 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	96	CYS	CB-SG	-6.90	1.70	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	65	LYS	CD-CE-NZ	-7.51	94.42	111.70
1	C	69	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	B	176	SER	CB-CA-C	-5.32	99.99	110.10
2	D	181	LEU	CA-CB-CG	5.17	127.19	115.30

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	1638	0	1581	37	0
1	C	1638	0	1581	47	0
2	B	1605	0	1565	34	0
2	D	1666	0	1619	31	0
3	E	163	0	149	6	0
3	G	163	0	149	2	0
4	F	229	0	218	6	0
4	H	222	0	209	3	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	61	0	0	5	0
6	B	88	0	0	11	0
6	C	77	0	0	8	0
6	D	115	0	0	7	0
6	E	8	0	0	0	0
6	F	10	0	0	0	0
6	G	15	0	0	1	0
6	H	5	0	0	0	0
All	All	7705	0	7071	157	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 11.

All (157) 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)
2:B:119:LYS:HD3	2:B:120:THR:N	1.68	1.07
1:A:42:LYS:O	6:A:301:HOH:O	1.79	0.99
1:A:70:ASP:OD2	6:A:302:HOH:O	1.83	0.95
1:C:24:LYS:HE2	1:C:69:ARG:HH21	1.34	0.91
3:E:12:SER:O	3:E:16:LEU:HD22	1.71	0.90
1:C:24:LYS:CE	1:C:69:ARG:HH21	1.89	0.85
1:C:97:PHE:O	6:C:301:HOH:O	1.98	0.81
1:A:135:LEU:HD11	1:A:145:VAL:HG22	1.64	0.80
2:B:39:GLN:OE1	6:B:301:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:MET:HG2	2:D:188:PRO:HA	1.64	0.80
2:B:119:LYS:HD3	2:B:120:THR:H	1.48	0.79
2:B:7:SER:OG	6:B:302:HOH:O	2.01	0.78
1:A:30:ASN:OD1	6:A:303:HOH:O	2.02	0.78
1:C:63:SER:OG	6:C:302:HOH:O	2.02	0.78
1:C:24:LYS:NZ	1:C:69:ARG:NH2	2.32	0.77
2:B:198:THR:HG22	2:B:213:LYS:HA	1.66	0.77
3:G:5:GLN:NE2	6:G:101:HOH:O	2.12	0.75
1:C:12:SER:OG	6:C:303:HOH:O	2.05	0.74
2:B:173:VAL:O	6:B:303:HOH:O	2.05	0.74
2:D:190:SER:O	6:D:301:HOH:O	2.06	0.73
1:A:179:THR:O	1:A:180:LEU:HD13	1.90	0.72
2:D:214:ILE:O	6:D:302:HOH:O	2.09	0.71
2:B:62:ASP:O	6:B:304:HOH:O	2.07	0.71
1:C:189:ASN:O	6:C:304:HOH:O	2.08	0.70
2:D:174:LEU:HD13	2:D:179:TYR:CE1	2.28	0.69
1:A:192:THR:HG23	1:A:207:SER:HB2	1.75	0.68
3:E:2:ILE:HG13	4:F:11:LEU:HD21	1.77	0.66
1:A:149:ILE:HA	1:A:190:SER:O	1.95	0.66
2:D:39:GLN:OE1	6:D:303:HOH:O	2.13	0.66
2:B:212:LYS:HD3	6:B:305:HOH:O	1.96	0.66
1:C:24:LYS:NZ	1:C:69:ARG:HH21	1.93	0.65
1:A:163:THR:HG22	1:A:164:ASP:O	1.97	0.65
2:B:211:ASP:O	6:B:305:HOH:O	2.13	0.65
1:C:90:GLN:HE21	1:C:92:ASP:H	1.45	0.64
2:D:157:THR:HG22	2:D:200:ASN:HB2	1.80	0.64
1:C:10:SER:OG	6:C:305:HOH:O	2.15	0.63
1:C:194:GLU:HG2	1:C:205:VAL:HG22	1.82	0.61
1:A:24:LYS:NZ	1:A:70:ASP:OD1	2.33	0.61
1:C:146:LYS:NZ	1:C:194:GLU:OE1	2.34	0.61
1:A:154:ARG:NH2	6:A:305:HOH:O	2.32	0.61
1:C:2:ILE:HD12	1:C:93:SER:HB3	1.83	0.60
2:B:42:GLU:OE2	2:B:44:ARG:NH2	2.32	0.60
1:C:9:SER:HB2	6:C:305:HOH:O	2.01	0.60
3:E:12:SER:O	3:E:16:LEU:CD2	2.47	0.60
2:B:196:THR:HB	2:B:213:LYS:HD2	1.84	0.59
1:A:112:PRO:HG2	1:A:204:ILE:HD12	1.85	0.58
2:B:125:VAL:HG22	2:B:146:VAL:HG12	1.84	0.58
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.86	0.57
1:A:80:PRO:O	1:A:83:VAL:HG22	2.05	0.57
1:C:61:ARG:HH12	1:C:82:ASP:CG	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:NE2	1:C:93:SER:H	2.02	0.57
1:A:119:PRO:HG3	1:A:129:ALA:HB1	1.87	0.56
2:D:200:ASN:HB3	6:D:311:HOH:O	2.05	0.56
1:C:61:ARG:NH1	1:C:82:ASP:OD1	2.38	0.56
1:C:90:GLN:HE21	1:C:92:ASP:N	2.04	0.56
2:D:51:ILE:HD13	2:D:72:ARG:HG3	1.87	0.56
1:A:150:ASP:OD1	1:A:188:HIS:HB3	2.06	0.55
1:C:24:LYS:HZ3	1:C:69:ARG:NH2	2.03	0.55
2:B:173:VAL:N	6:B:303:HOH:O	2.33	0.54
1:C:119:PRO:HG3	1:C:129:ALA:HB1	1.90	0.53
2:B:167:VAL:HA	2:B:184:SER:O	2.08	0.52
1:C:1:ASP:CG	1:C:2:ILE:H	2.12	0.52
4:F:14:ALA:O	4:F:18:VAL:HG23	2.08	0.52
1:C:162:TRP:CE2	1:C:174:MET:HG3	2.44	0.52
1:C:11:LEU:HB3	1:C:103:LEU:HD12	1.92	0.52
1:A:127:GLY:HA3	1:A:182:LYS:HE3	1.92	0.51
1:A:205:VAL:O	1:A:206:LYS:HG2	2.10	0.51
2:B:200:ASN:ND2	2:B:211:ASP:OD2	2.42	0.51
1:A:136:ASN:HB3	1:A:137:ASN:OD1	2.11	0.50
1:C:35:TRP:CE2	1:C:73:PHE:HB2	2.47	0.50
1:C:89:LEU:HD11	1:C:95:LEU:HD22	1.93	0.49
2:D:53:ASN:OD1	3:E:1:GLY:N	2.45	0.49
2:D:47:TRP:O	2:D:61:PRO:HG3	2.12	0.49
2:B:119:LYS:C	2:B:119:LYS:HD3	2.32	0.49
1:A:89:LEU:HD11	1:A:95:LEU:HD22	1.95	0.48
2:D:188:PRO:HB2	2:D:191:THR:HG23	1.96	0.48
2:D:19:LYS:HE3	6:D:308:HOH:O	2.12	0.48
1:C:12:SER:HA	1:C:104:GLU:O	2.13	0.47
2:D:145:LEU:CD2	2:D:147:LYS:HB2	2.44	0.47
1:A:107:ARG:HD2	1:A:170:SER:O	2.14	0.47
2:B:122:PRO:O	6:B:306:HOH:O	2.20	0.47
1:A:187:ARG:HB3	1:A:188:HIS:ND1	2.29	0.47
2:D:33:ASP:HB3	2:D:50:PHE:CE1	2.50	0.47
2:D:65:LYS:NZ	6:D:314:HOH:O	2.47	0.47
1:C:28:ASP:OD2	6:C:306:HOH:O	2.20	0.46
2:D:158:TRP:CZ3	2:D:199:CYS:HB3	2.50	0.46
1:A:107:ARG:NH1	1:A:110:ALA:HB2	2.31	0.46
3:G:2:ILE:HD11	4:H:15:LEU:HD21	1.97	0.46
2:B:158:TRP:CH2	2:B:199:CYS:HB3	2.51	0.45
1:A:205:VAL:C	1:A:206:LYS:HG2	2.35	0.45
1:C:24:LYS:HE3	1:C:70:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:HB2	2:B:104:PHE:HE1	1.81	0.45
1:C:186:GLU:HA	1:C:210:ARG:CZ	2.46	0.45
1:C:90:GLN:HE22	1:C:93:SER:H	1.65	0.45
2:B:63:THR:HG23	6:B:312:HOH:O	2.16	0.45
3:E:19:TYR:CE1	4:F:28:PRO:HD3	2.52	0.45
1:C:2:ILE:CD1	1:C:93:SER:HB3	2.47	0.44
2:D:122:PRO:HB3	2:D:208:THR:HG21	2.00	0.44
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.78	0.44
1:A:194:GLU:HG2	1:A:205:VAL:HG22	1.98	0.44
1:A:52:SER:HB3	1:A:64:GLY:O	2.18	0.44
2:D:127:PRO:O	2:D:128:LEU:HD23	2.18	0.44
2:D:168:HIS:HB2	2:D:184:SER:HB3	1.99	0.44
1:A:127:GLY:C	1:A:182:LYS:HB3	2.39	0.43
2:B:98:ARG:NH2	2:B:105:ASP:OD2	2.46	0.43
2:D:157:THR:CG2	2:D:200:ASN:HB2	2.48	0.43
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.53	0.43
2:D:29:PHE:CD1	2:D:77:ASN:HA	2.53	0.43
1:A:119:PRO:HB3	1:A:130:SER:H	1.83	0.43
2:B:124:SER:O	2:B:146:VAL:HA	2.19	0.43
2:B:44:ARG:CZ	2:B:44:ARG:HB2	2.49	0.43
2:B:83:MET:HB3	2:B:86(C):LEU:HD21	2.00	0.43
1:A:124:LEU:HD21	1:A:129:ALA:HB2	2.00	0.43
2:B:192:TRP:CG	2:B:193:PRO:HA	2.53	0.43
1:C:136:ASN:HB3	1:C:137:ASN:OD1	2.19	0.43
1:C:32:TYR:CE2	4:F:29:LYS:HD3	2.54	0.43
1:C:66:GLY:HA3	1:C:71:TYR:HA	2.01	0.43
1:A:107:ARG:O	6:A:304:HOH:O	2.20	0.42
2:B:119:LYS:CD	2:B:120:THR:H	2.25	0.42
2:B:148:GLY:HA2	2:B:178:LEU:HB3	2.00	0.42
2:D:86(C):LEU:HA	2:D:86(C):LEU:HD23	1.89	0.42
1:A:185:TYR:O	1:A:191:TYR:OH	2.36	0.42
2:B:157:THR:OG1	2:B:200:ASN:HB2	2.18	0.42
2:D:206:SER:OG	2:D:208:THR:HG23	2.19	0.42
2:D:69:THR:OG1	6:D:304:HOH:O	2.15	0.42
1:C:1:ASP:N	6:C:313:HOH:O	2.53	0.42
1:C:24:LYS:HZ1	1:C:69:ARG:NH2	2.12	0.42
1:C:61:ARG:CZ	1:C:79:GLU:HG3	2.50	0.42
2:B:185:VAL:HG22	2:B:187:VAL:HG13	2.01	0.42
2:B:62:ASP:N	6:B:312:HOH:O	2.53	0.42
2:D:42:GLU:H	2:D:42:GLU:CD	2.24	0.42
2:D:6:GLU:HG3	2:D:96:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:VAL:HA	2:D:184:SER:O	2.19	0.41
4:H:14:ALA:O	4:H:18:VAL:HG23	2.20	0.41
2:B:159:ASN:OD1	2:B:197:VAL:HA	2.20	0.41
1:C:55:GLN:HG3	1:C:56:PRO:HD2	2.01	0.41
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.55	0.41
3:E:18:ASN:O	4:F:29:LYS:HG2	2.20	0.41
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.87	0.41
2:D:1:GLU:O	2:D:26:GLY:HA3	2.20	0.41
1:A:13:ALA:O	1:A:106:LYS:N	2.40	0.41
1:C:10:SER:HA	1:C:102:LYS:O	2.20	0.41
1:A:32:TYR:CD2	4:H:29:LYS:HD2	2.55	0.41
2:B:203:HIS:HB3	2:B:208:THR:HB	2.02	0.41
1:A:107:ARG:HG2	1:A:139:TYR:CD2	2.55	0.41
1:A:187:ARG:HB3	1:A:188:HIS:CE1	2.56	0.41
1:C:95:LEU:HD23	1:C:95:LEU:HA	1.64	0.41
2:D:88:SER:HA	2:D:115:VAL:HB	2.02	0.41
1:A:139:TYR:CG	1:A:140:PRO:HA	2.56	0.41
1:A:127:GLY:CA	1:A:182:LYS:HE3	2.52	0.40
2:B:61:PRO:HB2	6:B:312:HOH:O	2.21	0.40
1:C:24:LYS:CE	1:C:69:ARG:NH2	2.68	0.40
1:C:35:TRP:CH2	1:C:88:CYS:HB3	2.56	0.40
1:C:92:ASP:HA	4:F:29:LYS:HE2	2.03	0.40
1:C:115:SER:O	1:C:133:CYS:HA	2.21	0.40
2:D:188:PRO:O	2:D:191:THR:OG1	2.17	0.40
1:C:118:PRO:HG2	2:D:217:ARG:CZ	2.51	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	209/213 (98%)	196 (94%)	13 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
2	B	206/220 (94%)	203 (98%)	2 (1%)	1 (0%)	29	41
2	D	217/220 (99%)	212 (98%)	4 (2%)	1 (0%)	29	41
3	E	19/21 (90%)	19 (100%)	0	0	100	100
3	G	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	F	27/30 (90%)	27 (100%)	0	0	100	100
4	H	26/30 (87%)	26 (100%)	0	0	100	100
All	All	932/968 (96%)	899 (96%)	31 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	177	ASP
2	D	132	SER

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	187/189 (99%)	177 (95%)	10 (5%)	22	37
1	C	187/189 (99%)	181 (97%)	6 (3%)	39	59
2	B	183/189 (97%)	179 (98%)	4 (2%)	52	71
2	D	189/189 (100%)	185 (98%)	4 (2%)	53	72
3	E	20/20 (100%)	18 (90%)	2 (10%)	7	11
3	G	20/20 (100%)	20 (100%)	0	100	100
4	F	24/25 (96%)	24 (100%)	0	100	100
4	H	23/25 (92%)	23 (100%)	0	100	100
All	All	833/846 (98%)	807 (97%)	26 (3%)	40	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	104	GLU
1	A	107	ARG
1	A	126	SER
1	A	141	LYS
1	A	148	LYS
1	A	161	SER
1	A	174	MET
1	A	182	LYS
1	A	187	ARG
2	B	162	SER
2	B	188	PRO
2	B	200	ASN
2	B	213	LYS
1	C	107	ARG
1	C	126	SER
1	C	152	SER
1	C	162	TRP
1	C	174	MET
1	C	182	LYS
2	D	7	SER
2	D	44	ARG
2	D	138	SER
2	D	218	ASP
3	E	9	SER
3	E	12	SER

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

Mol	Chain	Res	Type
1	C	90	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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, 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	211/213 (99%)	0.78	41 (19%) 1 0	32, 58, 110, 124	0
1	C	211/213 (99%)	-0.13	1 (0%) 91 89	34, 50, 66, 75	0
2	B	210/220 (95%)	0.14	8 (3%) 40 39	30, 48, 83, 91	0
2	D	218/220 (99%)	-0.13	4 (1%) 68 66	28, 38, 67, 98	0
3	E	21/21 (100%)	-0.15	0 100 100	33, 44, 55, 65	0
3	G	21/21 (100%)	-0.12	0 100 100	34, 41, 53, 60	0
4	F	29/30 (96%)	0.02	2 (6%) 16 15	36, 43, 70, 80	0
4	H	28/30 (93%)	-0.04	0 100 100	32, 44, 69, 83	0
All	All	949/968 (98%)	0.14	56 (5%) 22 21	28, 46, 95, 124	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	ASN	7.0
1	A	126	SER	5.2
1	A	180	LEU	5.1
1	A	201	THR	5.0
1	A	143	ILE	4.9
2	B	129	ALA	4.6
1	A	131	VAL	4.5
1	A	192	THR	4.4
1	A	191	TYR	4.4
2	D	134	ALA	4.0
1	A	154	ARG	3.9
2	D	133	ALA	3.9
1	A	181	THR	3.8
1	A	147	TRP	3.7
1	A	145	VAL	3.7
1	A	211	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	SER	3.6
1	A	149	ILE	3.4
2	D	132	SER	3.4
1	A	120	SER	3.4
1	A	207	SER	3.3
1	A	121	SER	3.3
1	A	116	ILE	3.3
1	A	155	GLN	3.3
1	A	209	ASN	3.2
1	A	204	ILE	3.1
1	A	208	PHE	3.1
1	A	179	THR	3.1
4	F	2	VAL	3.1
1	A	196	THR	3.0
2	B	187	VAL	2.9
1	A	183	ASP	2.9
1	A	132	VAL	2.8
1	C	181	THR	2.8
1	A	162	TRP	2.8
2	B	163	LEU	2.8
1	A	142	ASP	2.8
1	A	118	PRO	2.7
2	B	196	THR	2.7
2	B	162	SER	2.6
2	D	136	THR	2.6
1	A	152	SER	2.6
4	F	3	ASN	2.5
2	B	142	LEU	2.5
1	A	151	GLY	2.5
1	A	203	PRO	2.4
1	A	205	VAL	2.3
2	B	185	VAL	2.3
1	A	202	SER	2.2
1	A	200	SER	2.2
1	A	182	LYS	2.2
1	A	193	CYS	2.2
1	A	189	ASN	2.1
1	A	190	SER	2.1
2	B	166	GLY	2.1
1	A	144	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	MG	H	101	1/1	0.96	0.23	33,33,33,33	0
5	MG	F	101	1/1	0.97	0.25	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.