



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 07:51 AM EDT

PDB ID : 6Z7Y
Title : Human insulin in complex with the analytical antibody OXI-005 Fab
Authors : Johansson, E.
Deposited on : 2020-06-02
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

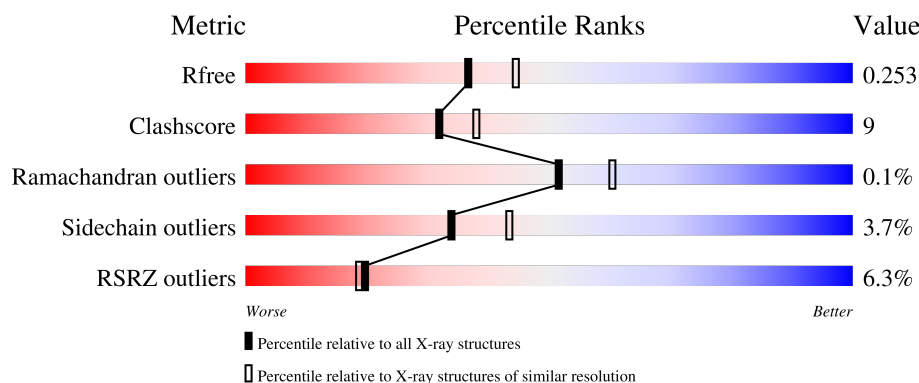
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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> <div>23%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
1	C	213	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
2	B	220	<div> <div>4%</div> <div>77%</div> <div>16%</div> <div>..</div> </div>
2	D	220	<div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
3	E	21	<div> <div>81%</div> <div>14%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	21	<div><div></div><div>76%</div><div>24%</div></div>
4	F	30	<div><div>3%</div><div></div><div>80%</div><div>17%</div><div></div><div></div></div>
4	H	30	<div><div></div><div>80%</div><div>10%</div><div></div><div>7%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7630 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
1	A	213	Total	C	N	O	S	0	0	0
			1654	1031	280	336	7			
1	C	211	Total	C	N	O	S	0	0	0
			1638	1023	278	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	1	0
			1622	1033	263	318	8			
2	D	209	Total	C	N	O	S	0	1	0
			1603	1023	257	315	8			

- Molecule 3 is a protein called Insulin.

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

- Molecule 4 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	29	Total	C	N	O	S	0	0	0
			231	149	39	41	2			
4	H	28	Total	C	N	O	S	0	0	0
			224	144	38	40	2			

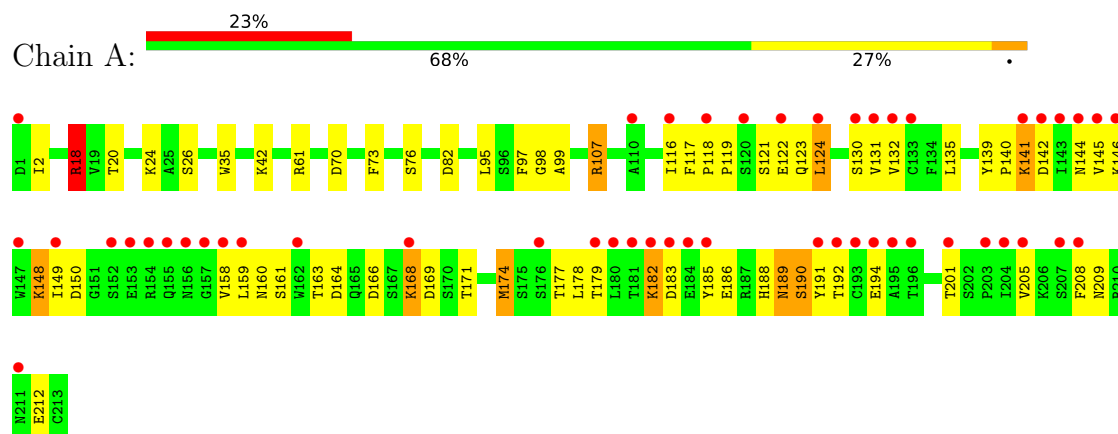
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total 52	O 52	0	0
5	B	70	Total 70	O 70	0	0
5	C	66	Total 66	O 66	0	0
5	D	106	Total 106	O 106	0	0
5	E	8	Total 8	O 8	0	0
5	F	9	Total 9	O 9	0	0
5	G	13	Total 13	O 13	0	0
5	H	8	Total 8	O 8	0	0

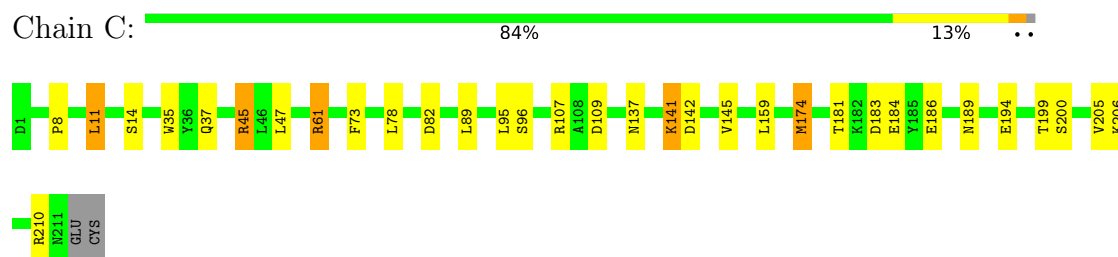
3 Residue-property plots

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.

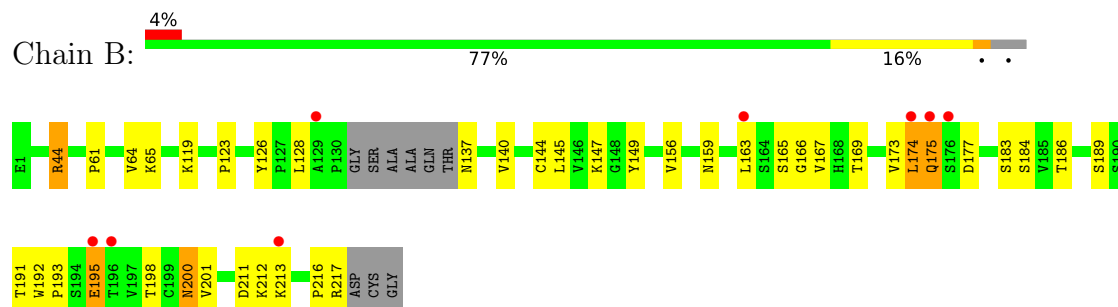
• Molecule 1: OXI-005 Fab Light chain



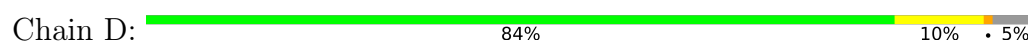
• Molecule 1: OXI-005 Fab Light chain



• Molecule 2: OXI-005 Fab Heavy chain

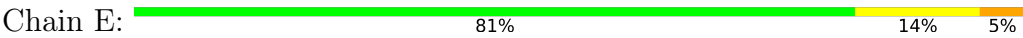


• Molecule 2: OXI-005 Fab Heavy chain

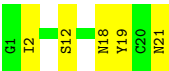




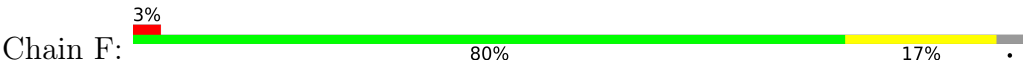
● Molecule 3: Insulin



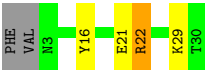
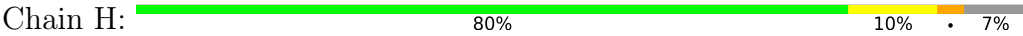
● Molecule 3: Insulin



● Molecule 4: Insulin



● Molecule 4: Insulin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.39Å 173.23Å 83.80Å 90.00° 135.83° 90.00°	Depositor
Resolution (Å)	48.42 – 2.20 48.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.42-2.20) 95.0 (48.42-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_3714	Depositor
R, R_{free}	0.217 , 0.253 0.217 , 0.253	Depositor DCC
R_{free} test set	1952 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7630	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

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	0.45	0/1692	0.80	7/2294 (0.3%)
1	C	0.47	0/1676	0.79	6/2274 (0.3%)
2	B	0.54	1/1665 (0.1%)	0.76	2/2274 (0.1%)
2	D	0.53	1/1646 (0.1%)	0.67	0/2249
3	E	0.51	0/164	0.70	0/220
3	G	0.57	0/164	0.67	0/220
4	F	0.52	0/237	0.56	0/319
4	H	0.56	0/230	0.72	1/309 (0.3%)
All	All	0.50	2/7474 (0.0%)	0.75	16/10159 (0.2%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	195	GLU	CB-CG	5.47	1.62	1.52
2	D	96	CYS	CB-SG	-5.45	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	C	45	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	18	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	C	11	LEU	CB-CG-CD1	-10.54	93.08	111.00
1	A	95	LEU	CA-CB-CG	9.28	136.64	115.30
1	A	168	LYS	CD-CE-NZ	8.11	130.36	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	GLN	CA-CB-CG	7.62	130.17	113.40
1	C	45	ARG	CD-NE-CZ	7.15	133.61	123.60
2	B	195	GLU	CA-CB-CG	7.02	128.84	113.40
1	C	11	LEU	CB-CG-CD2	6.80	122.56	111.00
1	A	183	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	18	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	95	LEU	CA-CB-CG	6.53	130.31	115.30
1	A	201	THR	C-N-CA	5.60	135.69	121.70
1	A	182	LYS	CB-CG-CD	5.35	125.50	111.60
4	H	21	GLU	N-CA-CB	-5.34	101.00	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	174	LEU	Peptide

5.2 Too-close contacts [i](#)

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	1654	0	1592	61	0
1	C	1638	0	1581	20	0
2	B	1622	0	1581	34	0
2	D	1603	0	1562	16	0
3	E	163	0	149	4	0
3	G	163	0	149	3	0
4	F	231	0	220	4	0
4	H	224	0	211	2	0
5	A	52	0	0	2	1
5	B	70	0	0	3	0
5	C	66	0	0	5	1
5	D	106	0	0	4	1
5	E	8	0	0	0	0
5	F	9	0	0	2	0
5	G	13	0	0	2	1
5	H	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7630	0	7045	128	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 9.

All (128) 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:124:LEU:HD23	1:A:182:LYS:HG2	1.37	1.02
1:A:61:ARG:NH1	1:A:82:ASP:OD1	1.93	1.01
1:A:61:ARG:HH12	1:A:82:ASP:CG	1.63	1.01
1:A:182:LYS:NZ	1:A:186:GLU:OE2	1.92	1.01
1:A:61:ARG:NH1	1:A:82:ASP:OD2	1.97	0.98
4:F:13:GLU:OE1	5:F:201:HOH:O	1.81	0.97
1:A:61:ARG:NH1	1:A:82:ASP:CG	2.21	0.94
4:F:4:GLN:O	5:F:202:HOH:O	1.93	0.85
1:A:116:ILE:HG22	5:A:314:HOH:O	1.79	0.83
3:E:12:SER:O	3:E:16:LEU:HD22	1.79	0.82
2:B:191:THR:O	2:B:195:GLU:HB2	1.81	0.81
2:D:123:PRO:O	5:D:301:HOH:O	2.03	0.75
1:A:182:LYS:NZ	1:A:186:GLU:CD	2.39	0.75
1:A:166:ASP:OD2	1:A:168:LYS:HB2	1.85	0.75
1:A:150:ASP:OD1	1:A:188:HIS:ND1	2.20	0.75
1:A:182:LYS:HZ1	1:A:186:GLU:CD	1.90	0.74
1:A:163:THR:HG22	1:A:164:ASP:O	1.89	0.73
3:G:21:ASN:O	5:G:101:HOH:O	2.08	0.71
3:E:12:SER:O	3:E:16:LEU:CD2	2.38	0.71
1:C:78:LEU:O	5:C:301:HOH:O	2.09	0.71
1:A:148:LYS:HB3	1:A:192:THR:HB	1.73	0.70
1:A:158:VAL:HG22	1:A:178:LEU:HD13	1.74	0.70
2:B:166:GLY:O	5:B:301:HOH:O	2.10	0.69
2:B:174:LEU:O	2:B:175:GLN:HB3	1.92	0.68
1:A:135:LEU:HD11	1:A:145:VAL:HG22	1.75	0.68
1:A:18:ARG:NH2	1:A:20:THR:OG1	2.27	0.68
2:D:216:PRO:O	5:D:302:HOH:O	2.11	0.67
2:B:137:ASN:N	5:B:303:HOH:O	2.29	0.66
1:C:189:ASN:ND2	5:C:306:HOH:O	2.28	0.66
2:D:19:LYS:O	5:D:303:HOH:O	2.13	0.65
5:G:101:HOH:O	4:H:22:ARG:NH1	2.18	0.65
1:A:212:GLU:HG2	2:B:217:ARG:HG3	1.80	0.64
1:C:8:PRO:HG2	1:C:11:LEU:HG	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD13	2:B:175:GLN:HA	1.79	0.63
1:A:70:ASP:OD2	5:A:301:HOH:O	2.15	0.63
1:A:99:ALA:HA	2:B:44:ARG:NE	2.14	0.62
2:D:188:PRO:HB2	2:D:191:THR:HG23	1.81	0.62
1:A:122:GLU:HG2	2:B:126:TYR:CE1	2.35	0.61
1:A:124:LEU:HD23	1:A:182:LYS:CG	2.20	0.61
1:A:123:GLN:NE2	1:A:130:SER:OG	2.31	0.60
2:B:198:THR:HG22	2:B:213:LYS:HA	1.82	0.60
1:C:181:THR:HG22	1:C:183:ASP:H	1.67	0.59
1:C:181:THR:HB	1:C:184:GLU:H	1.67	0.59
1:C:194:GLU:HG2	1:C:205:VAL:HG22	1.86	0.58
1:A:122:GLU:HB3	2:B:126:TYR:HD1	1.67	0.58
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.86	0.58
1:A:119:PRO:HD3	1:A:131:VAL:HG22	1.85	0.57
1:A:194:GLU:HB3	1:A:205:VAL:HG22	1.86	0.57
2:B:65:LYS:NZ	5:B:304:HOH:O	2.37	0.57
2:D:169:THR:HG22	2:D:183:SER:OG	2.05	0.57
1:C:89:LEU:HD12	1:C:96:SER:O	2.04	0.56
1:A:148:LYS:O	1:A:192:THR:N	2.36	0.56
1:A:98:GLY:O	2:B:44:ARG:NH2	2.39	0.56
1:C:141:LYS:HD3	1:C:142:ASP:H	1.69	0.56
1:A:124:LEU:CD2	1:A:182:LYS:HE2	2.36	0.55
2:B:200:ASN:ND2	2:B:211:ASP:OD1	2.30	0.54
1:A:144:ASN:HB3	1:A:146:LYS:HZ2	1.73	0.53
1:A:116:ILE:HG12	1:A:208:PHE:HD2	1.72	0.53
2:D:138:SER:N	5:D:312:HOH:O	2.41	0.53
1:A:182:LYS:NZ	1:A:186:GLU:OE1	2.41	0.53
1:A:97:PHE:HB2	2:B:44:ARG:HH22	1.73	0.53
3:G:2:ILE:HD12	3:G:19:TYR:CG	2.44	0.52
2:B:165:SER:C	2:B:167:VAL:H	2.13	0.52
1:A:61:ARG:HB2	1:A:76:SER:O	2.10	0.51
1:A:132:VAL:HG12	1:A:177:THR:HG23	1.92	0.51
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.46	0.51
1:A:159:LEU:HD13	2:B:173:VAL:HG11	1.93	0.51
1:A:24:LYS:NZ	1:A:70:ASP:OD1	2.33	0.51
1:A:124:LEU:HD23	1:A:182:LYS:HE2	1.92	0.51
2:D:125:VAL:HG12	2:D:212:LYS:HD2	1.93	0.51
1:C:137:ASN:O	5:C:302:HOH:O	2.19	0.50
1:C:61:ARG:NH1	1:C:82:ASP:OD1	2.40	0.50
1:A:169:ASP:N	1:A:169:ASP:OD1	2.44	0.49
1:A:145:VAL:C	1:A:146:LYS:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:HA	1:A:191:TYR:OH	2.13	0.49
1:C:199:THR:O	1:C:200:SER:HB2	2.12	0.49
1:A:117:PHE:HB2	1:A:132:VAL:CG2	2.43	0.48
2:D:174:LEU:HD13	2:D:179:TYR:CE1	2.49	0.48
1:A:2:ILE:HG23	1:A:26:SER:OG	2.14	0.48
2:B:166:GLY:HA3	2:B:186:THR:H	1.78	0.48
1:A:149:ILE:HA	1:A:190:SER:O	2.15	0.47
3:E:2:ILE:HD13	3:E:19:TYR:CG	2.49	0.47
1:C:109:ASP:HB3	1:C:199:THR:HG22	1.97	0.47
2:D:206:SER:OG	2:D:208:THR:HG22	2.15	0.47
2:B:167:VAL:HA	2:B:184:SER:O	2.15	0.46
2:D:174:LEU:HD13	2:D:179:TYR:CZ	2.50	0.46
2:B:156:VAL:HG12	2:B:201:VAL:HG22	1.99	0.45
1:A:149:ILE:HG22	1:A:150:ASP:OD1	2.17	0.45
2:B:61:PRO:HG2	2:B:64:VAL:HG22	1.98	0.45
1:A:107:ARG:HE	1:A:171:THR:HG22	1.81	0.45
1:A:177:THR:HG22	1:A:179:THR:HG23	1.99	0.44
1:A:132:VAL:HG21	2:B:128:LEU:HD13	1.99	0.44
2:B:44:ARG:NE	2:B:44:ARG:HA	2.33	0.44
1:C:145:VAL:HG21	1:C:174:MET:HE1	1.99	0.44
2:D:167:VAL:HA	2:D:184:SER:O	2.18	0.44
1:A:117:PHE:HB2	1:A:132:VAL:HG23	2.00	0.43
2:B:123:PRO:HB3	2:B:149:TYR:HB3	2.00	0.43
2:D:167:VAL:HG22	2:D:185:VAL:HG23	2.00	0.43
2:B:169:THR:HG23	2:B:183:SER:HB2	2.00	0.43
1:A:122:GLU:HB3	2:B:126:TYR:CD1	2.50	0.43
1:A:141:LYS:HG2	1:A:142:ASP:N	2.33	0.43
1:A:139:TYR:CG	1:A:140:PRO:HA	2.54	0.43
1:A:160:ASN:HB3	1:A:174:MET:HE2	2.00	0.43
2:B:192:TRP:CG	2:B:193:PRO:HA	2.54	0.43
3:E:2:ILE:HG13	4:F:11:LEU:HD21	2.00	0.43
1:A:119:PRO:HB2	1:A:124:LEU:HD11	2.00	0.42
1:A:122:GLU:OE1	2:B:212:LYS:HE2	2.19	0.42
1:C:141:LYS:HD2	5:C:335:HOH:O	2.19	0.42
1:C:35:TRP:CE2	1:C:73:PHE:HB2	2.55	0.42
1:A:191:TYR:HB2	1:A:208:PHE:CE2	2.55	0.42
2:D:42:GLU:OE1	2:D:42:GLU:N	2.47	0.42
2:D:196:THR:HG21	2:D:213:LYS:HG2	2.02	0.42
1:A:118:PRO:HG2	2:B:217:ARG:HH22	1.84	0.42
1:C:186:GLU:HA	1:C:210:ARG:CZ	2.50	0.42
1:C:159:LEU:HD11	2:D:175:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:HD3	1:C:206:LYS:HA	1.78	0.41
3:G:18:ASN:O	4:H:29:LYS:HG2	2.20	0.41
1:A:122:GLU:HG2	2:B:126:TYR:CD1	2.55	0.41
2:D:123:PRO:HD2	2:D:208:THR:HG21	2.01	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.58	0.41
1:A:189:ASN:O	1:A:209:ASN:HA	2.20	0.41
2:B:159:ASN:HB2	2:B:163:LEU:HG	2.02	0.41
1:A:212:GLU:CG	2:B:217:ARG:HG3	2.48	0.41
4:F:21:GLU:OE2	4:F:21:GLU:N	2.52	0.41
2:B:128:LEU:HG	2:B:144[A]:CYS:HA	2.04	0.40
2:B:145:LEU:HD22	2:B:147:LYS:HB2	2.02	0.40
2:B:140:VAL:HG23	2:B:189:SER:HA	2.04	0.40
1:C:206:LYS:NZ	5:C:316:HOH:O	2.54	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)
5:A:348:HOH:O	5:C:357:HOH:O[4_445]	1.94	0.26
5:D:398:HOH:O	5:G:110:HOH:O[1_556]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

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	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
1	C	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
2	B	208/220 (94%)	201 (97%)	6 (3%)	1 (0%)	29	31
2	D	206/220 (94%)	200 (97%)	6 (3%)	0	100	100
3	E	19/21 (90%)	19 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	925/968 (96%)	890 (96%)	34 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	PRO

5.3.2 Protein sidechains ⓘ

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	189/189 (100%)	178 (94%)	11 (6%)	20	23
1	C	187/189 (99%)	181 (97%)	6 (3%)	39	50
2	B	185/189 (98%)	181 (98%)	4 (2%)	52	65
2	D	183/189 (97%)	178 (97%)	5 (3%)	44	57
3	E	20/20 (100%)	19 (95%)	1 (5%)	24	30
3	G	20/20 (100%)	19 (95%)	1 (5%)	24	30
4	F	25/26 (96%)	24 (96%)	1 (4%)	31	40
4	H	24/26 (92%)	22 (92%)	2 (8%)	11	11
All	All	833/848 (98%)	802 (96%)	31 (4%)	34	43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	42	LYS
1	A	107	ARG
1	A	121	SER
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	141	LYS
1	A	148	LYS
1	A	161	SER
1	A	174	MET
1	A	189	ASN
1	A	190	SER
2	B	44	ARG
2	B	119	LYS
2	B	177	ASP
2	B	200	ASN
1	C	14	SER
1	C	45	ARG
1	C	61	ARG
1	C	107	ARG
1	C	141	LYS
1	C	174	MET
2	D	35	SER
2	D	199	CYS
2	D	200	ASN
2	D	212	LYS
2	D	213	LYS
3	E	12	SER
4	F	29	LYS
3	G	12	SER
4	H	16	TYR
4	H	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 monosaccharides 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, 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	213/213 (100%)	0.94	50 (23%) 0 0	37, 64, 119, 131	0
1	C	211/213 (99%)	-0.17	0 100 100	39, 56, 71, 86	0
2	B	211/220 (95%)	-0.01	8 (3%) 40 38	35, 51, 87, 100	0
2	D	209/220 (95%)	-0.24	0 100 100	33, 43, 67, 78	0
3	E	21/21 (100%)	-0.11	0 100 100	37, 51, 59, 64	0
3	G	21/21 (100%)	-0.07	0 100 100	37, 46, 58, 65	0
4	F	29/30 (96%)	0.08	1 (3%) 45 43	39, 48, 71, 91	0
4	H	28/30 (93%)	0.17	0 100 100	39, 48, 76, 78	0
All	All	943/968 (97%)	0.12	59 (6%) 20 19	33, 51, 104, 131	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLN	8.3
1	A	154	ARG	7.8
1	A	147	TRP	7.1
1	A	149	ILE	6.0
1	A	143	ILE	5.9
1	A	156	ASN	5.9
1	A	145	VAL	5.4
1	A	152	SER	5.4
1	A	181	THR	4.7
1	A	116	ILE	4.6
1	A	132	VAL	4.3
4	F	2	VAL	4.2
1	A	195	ALA	4.0
1	A	180	LEU	4.0
1	A	193	CYS	3.8
1	A	183	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	3.6
1	A	192	THR	3.5
1	A	146	LYS	3.5
1	A	144	ASN	3.4
1	A	142	ASP	3.3
1	A	179	THR	3.3
1	A	133	CYS	3.2
1	A	203	PRO	3.2
1	A	191	TYR	3.1
1	A	182	LYS	3.0
1	A	110	ALA	3.0
1	A	205	VAL	2.9
2	B	213	LYS	2.9
2	B	195	GLU	2.8
1	A	204	ILE	2.8
1	A	176	SER	2.8
1	A	153	GLU	2.8
1	A	131	VAL	2.7
1	A	158	VAL	2.7
1	A	196	THR	2.7
1	A	185	TYR	2.7
1	A	211	ASN	2.7
1	A	159	LEU	2.6
1	A	141	LYS	2.6
2	B	174	LEU	2.6
2	B	175	GLN	2.6
2	B	163	LEU	2.6
2	B	129	ALA	2.6
2	B	196	THR	2.4
1	A	162	TRP	2.4
1	A	201	THR	2.3
1	A	118	PRO	2.3
1	A	194	GLU	2.3
1	A	168	LYS	2.3
1	A	120	SER	2.3
1	A	1	ASP	2.2
1	A	207	SER	2.2
1	A	184	GLU	2.2
1	A	124	LEU	2.2
1	A	122	GLU	2.2
1	A	130	SER	2.1
2	B	176	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	208	PHE	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.