



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:34 am BST

PDB ID : 6EV1
Title : Crystal structure of antibody against schizophyllan
Authors : Sung, K.H.; Josewski, J.; Dubel, S.; Blankenfeldt, W.; Rau, U.
Deposited on : 2017-11-01
Resolution : 3.04 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

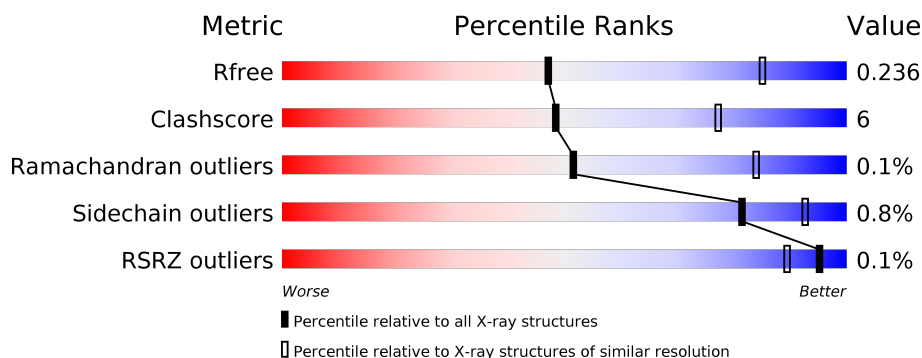
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 $\leq 5\%$. 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	220	
1	C	220	
1	E	220	
1	G	220	
1	I	220	
1	K	220	

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Mol	Chain	Length	Quality of chain
2	B	213	 85% 14%
2	D	213	 83% 15%
2	F	213	 87% 12%
2	H	213	 80% 18%
2	J	213	 84% 15%
2	L	213	 83% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19278 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 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1594	1015	256	316	7			
1	C	214	Total	C	N	O	S	0	0	0
			1617	1028	260	321	8			
1	E	211	Total	C	N	O	S	0	0	0
			1599	1019	257	316	7			
1	G	211	Total	C	N	O	S	0	0	0
			1597	1018	257	315	7			
1	I	205	Total	C	N	O	S	0	0	0
			1551	992	250	302	7			
1	K	218	Total	C	N	O	S	0	0	0
			1641	1042	265	327	7			

- Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1606	1002	269	327	8			
2	D	210	Total	C	N	O	S	0	0	0
			1606	1002	269	327	8			
2	F	212	Total	C	N	O	S	0	0	0
			1619	1009	271	331	8			
2	H	211	Total	C	N	O	S	0	0	0
			1610	1004	270	328	8			
2	J	212	Total	C	N	O	S	0	0	0
			1619	1009	271	331	8			
2	L	211	Total	C	N	O	S	0	0	0
			1610	1004	270	328	8			

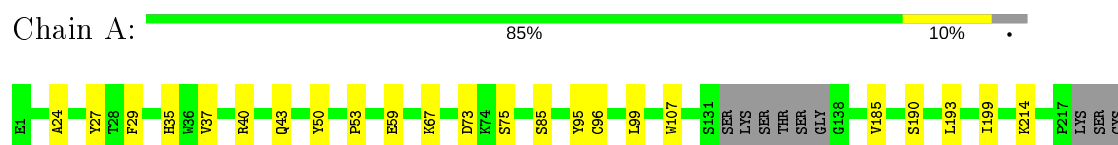
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0
3	C	2	Total 2	O 2	0	0
3	D	1	Total 1	O 1	0	0
3	E	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0
3	J	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0

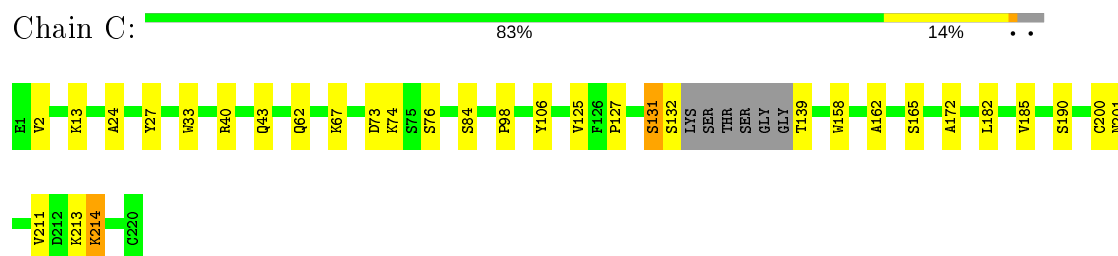
3 Residue-property plots [i](#)

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.

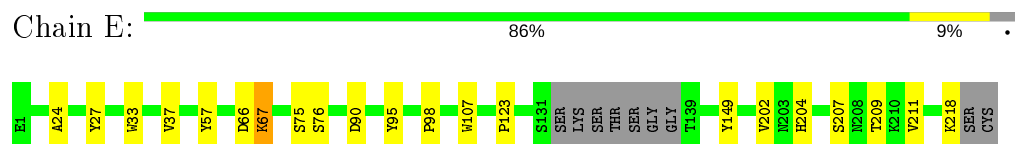
- Molecule 1: Heavy chain



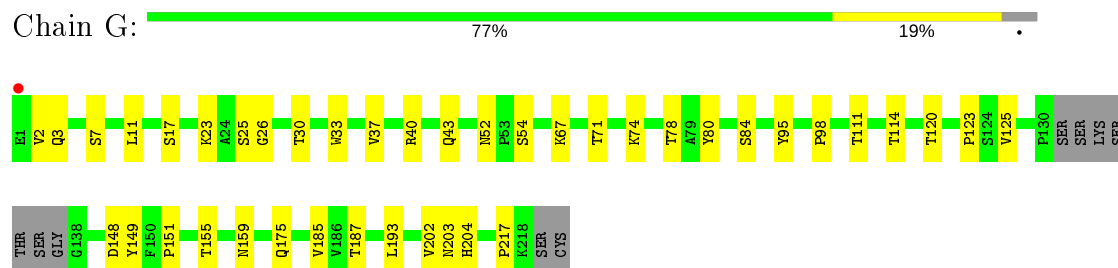
- Molecule 1: Heavy chain



- Molecule 1: Heavy chain

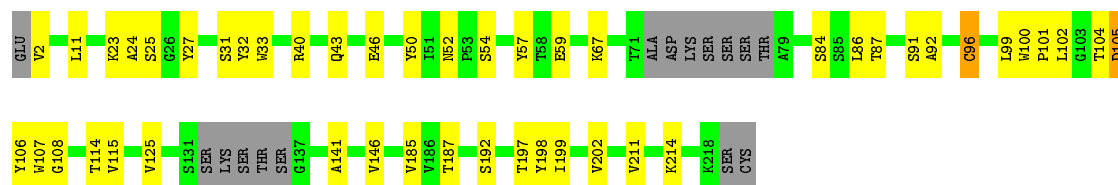


- Molecule 1: Heavy chain



- Molecule 1: Heavy chain





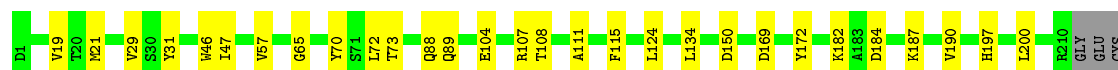
- Molecule 1: Heavy chain

Chain K: 86% 13%



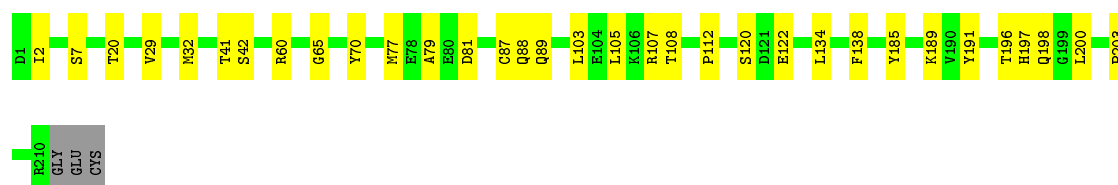
- Molecule 2: Light chain

Chain B: 85% 14%



- Molecule 2: Light chain

Chain D: 83% 15%



- Molecule 2: Light chain

Chain F: 87% 12%



- Molecule 2: Light chain

Chain H: 80% 18%



- Molecule 2: Light chain

Chain J:

84%

15%



● Molecule 2: Light chain

Chain L:

83%

16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.08 Å 112.83 Å 140.82 Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	56.42 – 3.04 139.23 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.4 (56.42-3.04) 99.4 (139.23-3.04)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.07 Å)	Xtriage
Refinement program	PHENIX (1.12rc1_2807: ???), REFMAC	Depositor
R, R_{free}	0.186 , 0.238 0.186 , 0.236	Depositor DCC
R_{free} test set	2692 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19278	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

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	0.31	0/1638	0.55	0/2237
1	C	0.32	0/1661	0.56	0/2267
1	E	0.30	0/1643	0.54	0/2243
1	G	0.31	0/1641	0.55	0/2240
1	I	0.30	0/1594	0.55	0/2175
1	K	0.33	0/1686	0.84	3/2301 (0.1%)
2	B	0.31	0/1643	0.55	0/2231
2	D	0.31	0/1643	0.54	0/2231
2	F	0.30	0/1656	0.54	1/2248 (0.0%)
2	H	0.36	1/1647 (0.1%)	0.58	3/2236 (0.1%)
2	J	0.30	0/1656	0.79	3/2248 (0.1%)
2	L	0.30	0/1647	0.53	0/2236
All	All	0.31	1/19755 (0.0%)	0.60	10/26893 (0.0%)

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	H	0	1
2	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	88	GLN	CB-CG	-6.38	1.35	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	62	GLN	CG-CD-OE1	22.63	166.87	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	36	GLN	CG-CD-OE1	19.01	159.61	121.60
1	K	62	GLN	CG-CD-NE2	-17.39	74.96	116.70
2	J	36	GLN	CG-CD-NE2	-16.88	76.18	116.70
1	K	62	GLN	OE1-CD-NE2	-8.46	102.44	121.90
2	J	36	GLN	OE1-CD-NE2	-7.44	104.79	121.90
2	H	88	GLN	CG-CD-NE2	-7.11	99.63	116.70
2	H	88	GLN	CB-CG-CD	5.46	125.78	111.60
2	H	88	GLN	CA-CB-CG	-5.35	101.64	113.40
2	F	178	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	88	GLN	Sidechain
2	J	36	GLN	Sidechain

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	1594	0	1549	13	0
1	C	1617	0	1574	21	1
1	E	1599	0	1559	15	0
1	G	1597	0	1557	25	0
1	I	1551	0	1511	31	0
1	K	1641	0	1601	17	0
2	B	1606	0	1555	18	1
2	D	1606	0	1555	22	0
2	F	1619	0	1564	14	0
2	H	1610	0	1558	29	0
2	J	1619	0	1564	20	0
2	L	1610	0	1558	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
All	All	19278	0	18705	228	1

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 6.

All (228) 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:D:32:MET:HE1	2:D:87:CYS:HB2	1.38	0.99
2:H:33:HIS:HB2	2:H:88:GLN:HG2	1.52	0.90
2:J:188:HIS:O	2:J:210:ARG:NH1	2.10	0.85
2:F:188:HIS:O	2:F:210:ARG:NH1	2.11	0.83
2:L:188:HIS:O	2:L:210:ARG:NH1	2.12	0.82
2:H:2:ILE:HD11	2:H:25:ALA:HB1	1.61	0.81
1:A:185:VAL:HG11	2:B:134:LEU:HD22	1.70	0.73
2:H:35:TYR:CE1	2:H:88:GLN:OE1	2.42	0.72
1:K:147:LYS:NZ	1:K:175:GLN:OE1	2.18	0.72
2:L:12:SER:HB2	2:L:106:LYS:HG3	1.71	0.70
2:D:32:MET:CE	2:D:87:CYS:HB2	2.18	0.69
1:E:123:PRO:HD2	1:E:209:THR:HG21	1.73	0.69
1:C:139:THR:N	1:C:190:SER:HG	1.92	0.68
2:H:35:TYR:HE1	2:H:88:GLN:OE1	1.75	0.68
1:I:23:LYS:NZ	1:I:25:SER:OG	2.25	0.68
2:J:104:GLU:OE1	2:J:172:TYR:OH	2.12	0.68
1:C:162:ALA:HA	1:C:165:SER:HB3	1.75	0.67
2:H:135:LEU:HD21	2:H:195:VAL:HG21	1.75	0.67
1:I:185:VAL:HG11	2:J:134:LEU:HD22	1.77	0.67
1:G:37:VAL:HG22	1:G:95:TYR:HB2	1.75	0.66
1:G:185:VAL:HG11	2:H:134:LEU:HD22	1.75	0.66
1:C:214:LYS:H	1:C:214:LYS:HD3	1.61	0.66
1:I:57:TYR:HE2	1:I:59:GLU:HG3	1.61	0.66
1:I:100:TRP:CD2	1:I:101:PRO:HA	2.31	0.65
1:E:204:HIS:HB3	1:E:209:THR:HG23	1.78	0.65
2:H:33:HIS:HB2	2:H:88:GLN:CG	2.25	0.65
2:L:60:ARG:NH2	2:L:80:GLU:OE2	2.29	0.65
1:A:37:VAL:HG22	1:A:95:TYR:HB2	1.78	0.64
1:C:139:THR:N	1:C:190:SER:OG	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:HA	1:A:193:LEU:HD13	1.79	0.63
2:F:104:GLU:OE2	2:F:141:ARG:NH2	2.32	0.63
1:I:32:TYR:HA	1:I:101:PRO:HD2	1.80	0.63
2:J:36:GLN:HG3	2:J:85:TYR:CE1	2.34	0.63
2:L:65:GLY:HA3	2:L:70:TYR:HA	1.82	0.62
2:H:154:GLN:OE1	2:H:157:ASN:ND2	2.31	0.62
1:K:148:ASP:OD1	1:K:175:GLN:NE2	2.29	0.62
2:L:107:ARG:NH1	2:L:108:THR:O	2.32	0.62
2:D:60:ARG:NH1	2:D:81:ASP:OD2	2.34	0.61
2:D:65:GLY:HA3	2:D:70:TYR:HA	1.83	0.61
1:C:185:VAL:HG11	2:D:134:LEU:HD22	1.83	0.61
1:C:2:VAL:HG13	1:C:106:TYR:HD2	1.67	0.60
2:J:65:GLY:HA3	2:J:70:TYR:HA	1.83	0.60
1:E:37:VAL:HG22	1:E:95:TYR:HB2	1.83	0.60
1:I:192:SER:HG	1:I:198:TYR:HH	1.48	0.60
1:I:87:THR:O	1:I:115:VAL:HG21	2.02	0.59
1:G:148:ASP:OD1	1:G:175:GLN:NE2	2.28	0.59
1:K:190:SER:HA	1:K:193:LEU:HD12	1.85	0.58
2:H:107:ARG:NH1	2:H:169:ASP:O	2.36	0.58
1:I:2:VAL:HG12	1:I:27:TYR:HB3	1.85	0.58
2:F:18:LYS:HG3	2:F:75:SER:HA	1.86	0.57
2:B:107:ARG:HG2	2:B:108:THR:N	2.19	0.57
2:D:107:ARG:NH1	2:D:108:THR:O	2.37	0.57
1:G:187:THR:HG21	2:H:136:ASN:ND2	2.21	0.56
2:J:212:GLU:OE1	2:J:212:GLU:N	2.33	0.56
2:J:107:ARG:HH21	2:J:110:ALA:HB2	1.71	0.55
2:D:196:THR:HG22	2:D:203:PRO:HB3	1.88	0.55
1:G:7:SER:O	1:G:111:THR:HG22	2.06	0.55
1:G:67:LYS:HE2	1:G:84:SER:O	2.06	0.55
1:C:67:LYS:HE2	1:C:84:SER:O	2.07	0.54
1:K:133:LYS:NZ	2:L:207:SER:O	2.19	0.54
2:B:29:VAL:O	2:B:70:TYR:OH	2.23	0.54
1:K:11:LEU:HD23	1:K:120:THR:HG22	1.90	0.54
2:H:65:GLY:HA3	2:H:70:TYR:HA	1.89	0.54
1:I:96:CYS:O	1:I:108:GLY:N	2.40	0.54
2:B:150:ASP:OD1	2:B:190:VAL:HG12	2.08	0.54
1:G:30:THR:HG21	1:G:74:LYS:HE3	1.90	0.53
1:I:104:THR:O	1:I:106:TYR:HD1	1.91	0.53
2:H:107:ARG:HG2	2:H:108:THR:N	2.23	0.53
1:A:73:ASP:OD1	1:A:75:SER:OG	2.26	0.53
1:G:123:PRO:HB3	1:G:149:TYR:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:SER:OG	1:C:132:SER:N	2.41	0.53
1:E:204:HIS:HB3	1:E:209:THR:CG2	2.38	0.53
2:J:107:ARG:NH2	2:J:110:ALA:HB2	2.23	0.52
1:K:37:VAL:HG22	1:K:95:TYR:HB2	1.91	0.52
2:F:120:SER:HB2	2:F:122:GLU:OE1	2.09	0.52
2:B:111:ALA:HB1	2:B:200:LEU:HD13	1.91	0.52
1:I:86:LEU:HB3	1:I:115:VAL:HG11	1.90	0.52
1:I:40:ARG:HG2	1:I:92:ALA:HB2	1.91	0.52
2:F:21:MET:SD	2:F:101:THR:OG1	2.65	0.52
1:I:52:ASN:OD1	1:I:54:SER:OG	2.15	0.52
2:B:184:ASP:HA	2:B:187:LYS:HE2	1.92	0.51
2:D:120:SER:HB2	2:D:122:GLU:OE1	2.09	0.51
1:G:11:LEU:HD23	1:G:120:THR:HG22	1.91	0.51
1:E:202:VAL:HB	1:E:211:VAL:HG13	1.93	0.51
2:B:124:LEU:HD22	2:B:182:LYS:HG3	1.91	0.51
2:L:184:ASP:OD1	2:L:187:LYS:NZ	2.44	0.51
2:B:88:GLN:HG2	2:B:89:GLN:N	2.27	0.50
1:K:11:LEU:HD12	1:K:114:THR:O	2.12	0.50
2:B:197:HIS:HB3	2:B:200:LEU:CD2	2.41	0.50
2:D:32:MET:HG3	2:D:70:TYR:CG	2.47	0.50
2:L:185:TYR:HA	2:L:191:TYR:OH	2.12	0.50
2:D:197:HIS:HB3	2:D:200:LEU:CD2	2.42	0.49
2:B:65:GLY:HA3	2:B:70:TYR:HA	1.94	0.49
1:G:193:LEU:HD13	1:G:217:PRO:HG2	1.95	0.49
1:C:125:VAL:HG21	1:C:211:VAL:HG11	1.94	0.49
1:I:91:SER:OG	1:I:115:VAL:HG22	2.12	0.49
2:L:79:ALA:HA	2:L:105:LEU:HD11	1.94	0.49
1:E:123:PRO:HB3	1:E:149:TYR:HB3	1.95	0.49
2:H:49:ASP:O	2:H:50:THR:OG1	2.30	0.49
2:H:12:SER:HB2	2:H:106:LYS:HG3	1.94	0.48
2:L:183:ALA:O	2:L:186:GLU:HG2	2.13	0.48
1:G:3:GLN:HG3	1:G:25:SER:HB2	1.95	0.48
1:I:24:ALA:HB1	1:I:27:TYR:CE2	2.48	0.48
2:F:88:GLN:HG2	2:F:89:GLN:N	2.27	0.48
2:D:20:THR:O	2:L:155:SER:OG	2.32	0.48
2:F:65:GLY:HA3	2:F:70:TYR:HA	1.94	0.48
1:K:33:TRP:O	1:K:98:PRO:HA	2.14	0.48
2:F:76:SER:OG	2:F:76:SER:O	2.31	0.48
1:I:202:VAL:N	1:I:211:VAL:O	2.42	0.48
1:G:52:ASN:OD1	1:G:54:SER:OG	2.23	0.47
2:L:115:PHE:HD2	2:L:134:LEU:HD23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:VAL:HG23	2:H:26:SER:HB3	1.96	0.47
2:H:48:TYR:CZ	2:H:52:LYS:HG2	2.49	0.47
2:H:35:TYR:CZ	2:H:88:GLN:OE1	2.67	0.47
2:B:107:ARG:NH1	2:B:169:ASP:O	2.48	0.47
1:G:23:LYS:HG3	1:G:78:THR:HG22	1.96	0.47
1:A:50:TYR:CE1	1:A:59:GLU:HB2	2.49	0.47
2:D:79:ALA:HA	2:D:105:LEU:HD21	1.97	0.47
1:K:192:SER:O	1:K:196:GLN:HB2	2.13	0.47
2:F:196:THR:HG22	2:F:203:PRO:HB3	1.96	0.47
2:H:21:MET:HE1	2:H:85:TYR:HB2	1.95	0.47
1:I:100:TRP:CZ3	1:I:102:LEU:HD23	2.50	0.47
2:F:147:TRP:CE2	2:F:178:LEU:HB2	2.50	0.47
1:I:99:LEU:HD11	1:I:107:TRP:NE1	2.30	0.47
2:D:88:GLN:HG2	2:D:89:GLN:N	2.29	0.46
2:L:147:TRP:CE2	2:L:178:LEU:HB2	2.50	0.46
1:C:74:LYS:NZ	1:G:17:SER:O	2.30	0.46
2:J:30:SER:N	2:J:91:SER:OG	2.33	0.46
1:G:125:VAL:HG11	1:G:202:VAL:HG21	1.97	0.46
2:H:141:ARG:NH2	2:H:172:TYR:OH	2.48	0.46
2:H:29:VAL:HG12	2:H:91:SER:HB2	1.97	0.46
1:I:31:SER:O	1:I:101:PRO:HG2	2.16	0.46
1:E:207:SER:OG	1:E:209:THR:HG22	2.15	0.46
2:D:107:ARG:HH11	2:D:107:ARG:HG2	1.80	0.46
2:H:72:LEU:HD12	2:H:73:THR:H	1.81	0.46
2:H:35:TYR:OH	2:H:88:GLN:OE1	2.22	0.46
2:B:197:HIS:HB3	2:B:200:LEU:HD22	1.98	0.46
2:F:60:ARG:NH2	2:F:80:GLU:OE2	2.46	0.46
2:B:47:ILE:HD12	2:B:72:LEU:HD13	1.98	0.45
1:A:29:PHE:CE2	1:A:53:PRO:HB3	2.50	0.45
2:F:77:MET:SD	2:F:103:LEU:HD21	2.57	0.45
1:C:158:TRP:CH2	1:C:200:CYS:HB3	2.52	0.45
1:G:187:THR:HG21	2:H:136:ASN:HD22	1.80	0.45
1:C:62:GLN:HB3	1:E:57:TYR:CD2	2.52	0.45
1:E:33:TRP:O	1:E:98:PRO:HA	2.17	0.45
1:I:11:LEU:HD12	1:I:114:THR:O	2.17	0.45
1:I:125:VAL:HG22	1:I:146:VAL:HG12	1.98	0.45
2:J:184:ASP:HA	2:J:187:LYS:NZ	2.31	0.45
1:K:135:THR:HG22	1:K:140:ALA:HB2	1.99	0.45
1:C:62:GLN:HB3	1:E:57:TYR:CE2	2.52	0.45
1:I:105:ASP:HB3	2:J:45:ARG:HB3	1.98	0.45
2:H:149:VAL:HG13	2:H:191:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:VAL:CG1	1:C:106:TYR:HD2	2.29	0.45
1:C:127:PRO:HD3	1:C:213:LYS:HE3	1.99	0.45
2:D:77:MET:SD	2:D:103:LEU:HD21	2.57	0.45
1:I:197:THR:HG23	1:I:214:LYS:HE3	1.99	0.45
1:I:40:ARG:NH2	1:I:43:GLN:HG2	2.32	0.45
2:L:29:VAL:HG12	2:L:91:SER:HB2	1.97	0.45
2:D:112:PRO:HB3	2:D:138:PHE:HB3	1.98	0.45
1:E:75:SER:OG	1:E:76:SER:N	2.50	0.45
1:I:187:THR:HG21	2:J:136:ASN:ND2	2.32	0.45
1:E:24:ALA:HB1	1:E:27:TYR:CE2	2.52	0.44
1:I:40:ARG:NH1	1:I:46:GLU:OE2	2.50	0.44
1:A:199:ILE:HG12	1:A:214:LYS:HA	2.00	0.44
2:J:107:ARG:HD2	2:J:169:ASP:O	2.17	0.44
1:G:40:ARG:NH2	1:G:43:GLN:HG2	2.32	0.44
1:K:170:PHE:CE2	2:L:163:THR:HG23	2.53	0.44
1:C:73:ASP:OD2	1:C:76:SER:OG	2.24	0.44
2:J:1:ASP:N	2:J:94:PRO:HD2	2.32	0.44
1:K:175:GLN:HA	2:L:159:GLN:OE1	2.18	0.44
2:B:46:TRP:CE2	2:B:57:VAL:HG13	2.53	0.43
1:G:2:VAL:HA	1:G:26:GLY:HA3	2.00	0.43
1:A:67:LYS:NZ	1:A:85:SER:O	2.51	0.43
2:B:115:PHE:CD1	2:B:134:LEU:HD23	2.53	0.43
1:I:50:TYR:CE1	1:I:59:GLU:HB2	2.54	0.43
1:G:155:THR:OG1	1:G:203:ASN:HB3	2.18	0.43
2:H:135:LEU:HD21	2:H:195:VAL:CG2	2.46	0.43
1:K:24:ALA:HB1	1:K:27:TYR:CE2	2.53	0.43
1:A:40:ARG:NH2	1:A:43:GLN:HG2	2.32	0.43
2:D:185:TYR:O	2:D:191:TYR:OH	2.30	0.43
1:G:151:PRO:O	1:G:204:HIS:NE2	2.32	0.43
2:H:72:LEU:HD12	2:H:73:THR:N	2.34	0.43
1:A:185:VAL:HG11	2:B:134:LEU:CD2	2.44	0.43
1:A:35:HIS:HB2	1:A:99:LEU:CD2	2.49	0.43
2:F:33:HIS:O	2:F:87:CYS:HA	2.18	0.43
1:G:33:TRP:O	1:G:98:PRO:HA	2.18	0.43
2:H:46:TRP:CE2	2:H:57:VAL:HG13	2.54	0.43
1:E:67:LYS:HD3	1:E:90:ASP:OD1	2.18	0.43
1:K:123:PRO:HB3	1:K:149:TYR:HB3	2.01	0.43
1:A:24:ALA:HB1	1:A:27:TYR:CE2	2.54	0.43
1:G:11:LEU:HD12	1:G:114:THR:O	2.18	0.43
1:I:33:TRP:H	1:I:101:PRO:HD2	1.84	0.43
2:J:185:TYR:CZ	2:J:210:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LEU:HD22	1:G:151:PRO:HD3	2.01	0.42
1:E:66:ASP:OD1	1:E:66:ASP:N	2.45	0.42
1:A:37:VAL:HG21	1:A:107:TRP:CZ3	2.54	0.42
1:K:135:THR:HG22	1:K:140:ALA:CB	2.48	0.42
2:F:46:TRP:CE2	2:F:57:VAL:HG13	2.55	0.42
1:C:13:LYS:HB3	1:C:13:LYS:HE2	1.83	0.42
1:I:67:LYS:HE2	1:I:84:SER:O	2.19	0.42
2:J:34:TRP:HB2	2:J:47:ILE:HB	2.00	0.42
2:J:150:ASP:OD1	2:J:190:VAL:HG12	2.19	0.42
1:C:33:TRP:O	1:C:98:PRO:HA	2.19	0.42
2:L:54:ALA:O	2:L:57:VAL:HG23	2.19	0.42
2:B:19:VAL:O	2:B:73:THR:HA	2.20	0.42
2:H:112:PRO:HB3	2:H:138:PHE:HB3	2.01	0.42
2:H:21:MET:HE1	2:H:101:THR:OG1	2.19	0.42
1:G:11:LEU:HB2	1:G:151:PRO:HG3	2.02	0.41
1:E:37:VAL:HG21	1:E:107:TRP:HZ3	1.85	0.41
2:D:107:ARG:HG2	2:D:107:ARG:NH1	2.35	0.41
2:D:29:VAL:O	2:D:70:TYR:OH	2.33	0.41
2:D:2:ILE:HD13	2:D:29:VAL:HG12	2.03	0.41
1:C:24:ALA:HB1	1:C:27:TYR:CE2	2.56	0.41
2:J:137:ASN:HA	2:J:171:THR:HB	2.03	0.41
2:J:44:LYS:HB2	2:J:44:LYS:HE3	1.76	0.41
1:G:71:THR:OG1	1:G:80:TYR:HB2	2.21	0.41
1:K:131:SER:O	1:K:135:THR:HG23	2.21	0.41
1:I:199:ILE:HG12	1:I:214:LYS:HA	2.02	0.41
2:J:21:MET:SD	2:J:101:THR:OG1	2.70	0.41
1:K:67:LYS:HE2	1:K:84:SER:O	2.21	0.41
2:B:104:GLU:OE1	2:B:172:TYR:OH	2.37	0.41
1:C:172:ALA:HA	1:C:182:LEU:HB3	2.03	0.41
2:D:32:MET:HG3	2:D:70:TYR:CD1	2.56	0.41
1:I:141:ALA:HB2	1:I:187:THR:HG22	2.03	0.40
1:C:40:ARG:HB2	1:C:43:GLN:HB2	2.02	0.40
2:D:41:THR:HG22	2:D:42:SER:H	1.87	0.40
2:L:33:HIS:O	2:L:87:CYS:HA	2.22	0.40
2:L:8:PRO:O	2:L:101:THR:HG23	2.22	0.40

All (1) 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:B:31:TYR:OH	1:C:201:ASN:ND2[2_646]	2.09	0.11

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	207/220 (94%)	204 (99%)	3 (1%)	0	100	100
1	C	210/220 (96%)	204 (97%)	6 (3%)	0	100	100
1	E	207/220 (94%)	199 (96%)	8 (4%)	0	100	100
1	G	207/220 (94%)	202 (98%)	4 (2%)	1 (0%)	29	65
1	I	199/220 (90%)	192 (96%)	6 (3%)	1 (0%)	29	65
1	K	216/220 (98%)	211 (98%)	5 (2%)	0	100	100
2	B	208/213 (98%)	201 (97%)	7 (3%)	0	100	100
2	D	208/213 (98%)	201 (97%)	7 (3%)	0	100	100
2	F	210/213 (99%)	202 (96%)	8 (4%)	0	100	100
2	H	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
2	J	210/213 (99%)	202 (96%)	8 (4%)	0	100	100
2	L	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	2500/2598 (96%)	2421 (97%)	77 (3%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	159	ASN
1	I	105	ASP

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	179/187 (96%)	178 (99%)	1 (1%)	86	94
1	C	183/187 (98%)	181 (99%)	2 (1%)	73	90
1	E	180/187 (96%)	178 (99%)	2 (1%)	73	90
1	G	179/187 (96%)	179 (100%)	0	100	100
1	I	173/187 (92%)	172 (99%)	1 (1%)	86	94
1	K	185/187 (99%)	181 (98%)	4 (2%)	52	79
2	B	183/185 (99%)	182 (100%)	1 (0%)	88	95
2	D	183/185 (99%)	180 (98%)	3 (2%)	62	85
2	F	184/185 (100%)	184 (100%)	0	100	100
2	H	183/185 (99%)	182 (100%)	1 (0%)	88	95
2	J	184/185 (100%)	181 (98%)	3 (2%)	62	85
2	L	183/185 (99%)	183 (100%)	0	100	100
All	All	2179/2232 (98%)	2161 (99%)	18 (1%)	81	92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	CYS
2	B	21	MET
1	C	131	SER
1	C	214	LYS
2	D	7	SER
2	D	189	LYS
2	D	198	GLN
1	E	67	LYS
1	E	218	LYS
2	H	194	GLU
1	I	96	CYS
2	J	30	SER
2	J	48	TYR
2	J	93	ASN
1	K	10	GLU
1	K	62	GLN
1	K	96	CYS
1	K	218	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	K	62	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	211/220 (95%)	-0.35	0 100 100	30, 61, 90, 109	0
1	C	214/220 (97%)	-0.35	0 100 100	21, 49, 91, 135	0
1	E	211/220 (95%)	-0.15	0 100 100	34, 72, 110, 141	0
1	G	211/220 (95%)	-0.25	1 (0%) 91 75	29, 56, 100, 132	0
1	I	205/220 (93%)	-0.22	0 100 100	38, 78, 129, 152	0
1	K	218/220 (99%)	-0.32	0 100 100	33, 61, 103, 125	0
2	B	210/213 (98%)	-0.40	0 100 100	26, 57, 87, 113	0
2	D	210/213 (98%)	-0.49	0 100 100	29, 59, 88, 100	0
2	F	212/213 (99%)	-0.40	1 (0%) 91 75	28, 66, 103, 125	0
2	H	211/213 (99%)	-0.37	0 100 100	35, 71, 98, 114	0
2	J	212/213 (99%)	-0.31	0 100 100	37, 78, 127, 144	0
2	L	211/213 (99%)	-0.32	1 (0%) 91 75	35, 66, 110, 134	0
All	All	2536/2598 (97%)	-0.33	3 (0%) 95 89	21, 64, 106, 152	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	ASP	3.4
1	G	1	GLU	2.4
2	L	128	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.