



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:07 AM GMT

PDB ID : 3QA3
Title : Crystal Structure of A-domain in complex with antibody
Authors : Mahalingam, B.; Xiong, J.P.; Arnaout, M.A.
Deposited on : 2011-01-10
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

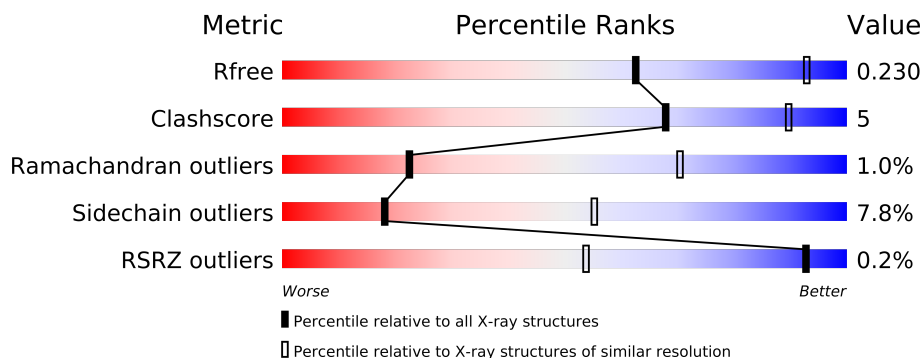
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	220	
1	C	220	
1	F	220	
1	J	220	
2	B	224	
2	D	224	
2	H	224	
2	K	224	
3	E	190	
3	G	190	
3	I	190	
3	L	190	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	C	221	-	X
4	EDO	D	2	-	X
4	EDO	J	221	-	X
4	EDO	J	222	-	X
4	EDO	K	227	-	X
5	GOL	B	1	-	X
5	GOL	D	227	-	X
5	GOL	G	5	-	X
5	GOL	G	6	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19772 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Antibody Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	A	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	F	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	J	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	B	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	H	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	K	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			

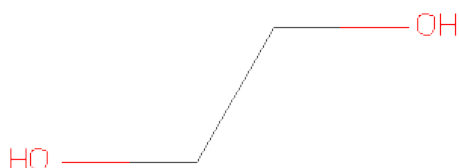
- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	187	Total	C	N	O	S	0	0	0
			1510	960	269	278	3			
3	E	186	Total	C	N	O	S	0	0	0
			1505	957	268	277	3			
3	I	185	Total	C	N	O	S	0	0	0
			1494	948	267	276	3			
3	L	185	Total	C	N	O	S	0	0	0
			1494	948	267	276	3			

There are 4 discrepancies between the modelled and reference sequences:

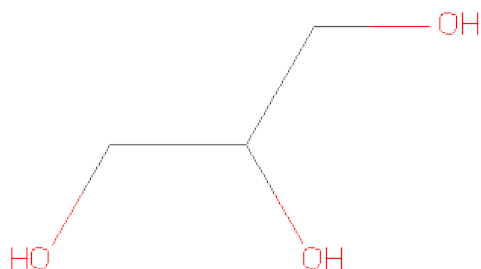
Chain	Residue	Modelled	Actual	Comment	Reference
G	316	GLY	ILE	ENGINEERED MUTATION	UNP P11215
E	316	GLY	ILE	ENGINEERED MUTATION	UNP P11215
I	316	GLY	ILE	ENGINEERED MUTATION	UNP P11215
L	316	GLY	ILE	ENGINEERED MUTATION	UNP P11215

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Ca	0	0
			1	1		
6	I	1	Total	Ca	0	0
			1	1		
6	L	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

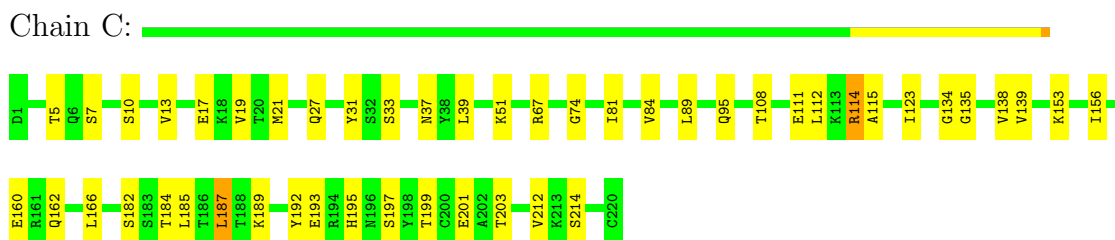
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	9	Total O 9 9	0	0
7	D	5	Total O 5 5	0	0
7	G	4	Total O 4 4	0	0
7	A	2	Total O 2 2	0	0
7	B	8	Total O 8 8	0	0
7	E	6	Total O 6 6	0	0
7	F	8	Total O 8 8	0	0
7	H	6	Total O 6 6	0	0
7	I	3	Total O 3 3	0	0
7	J	9	Total O 9 9	0	0
7	K	10	Total O 10 10	0	0
7	L	5	Total O 5 5	0	0

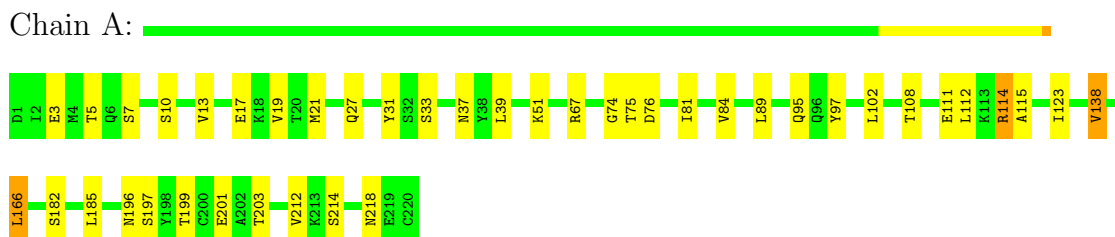
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

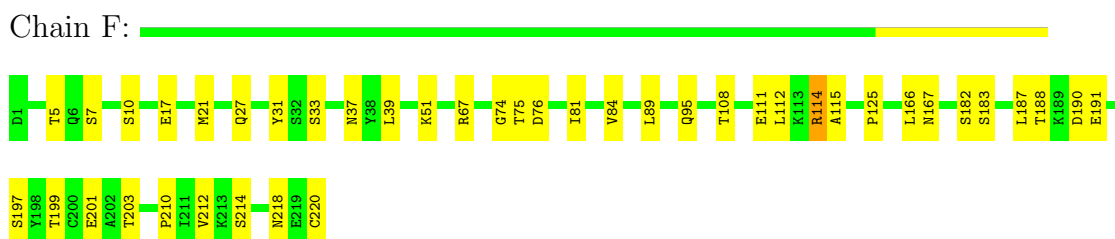
- Molecule 1: Antibody Light chain



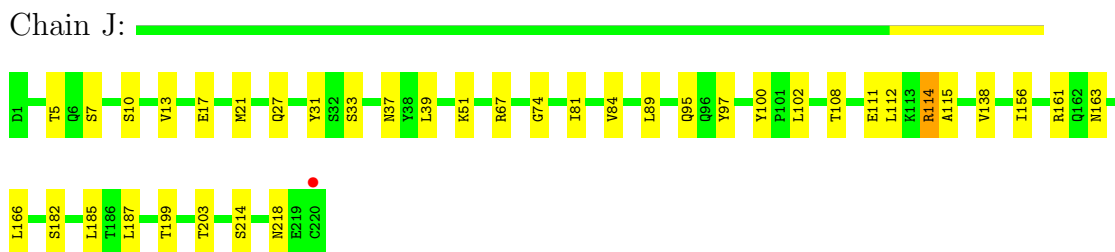
- Molecule 1: Antibody Light chain



- Molecule 1: Antibody Light chain



- Molecule 1: Antibody Light chain



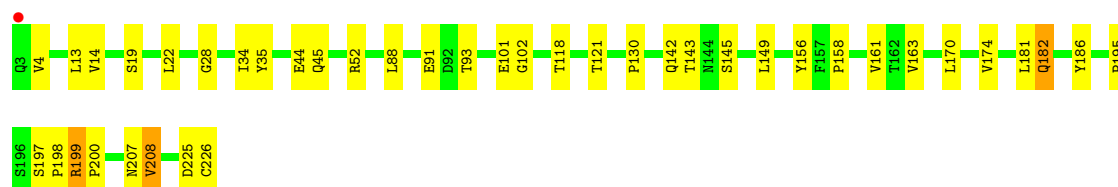
- Molecule 2: Antibody Heavy chain

Chain D: 



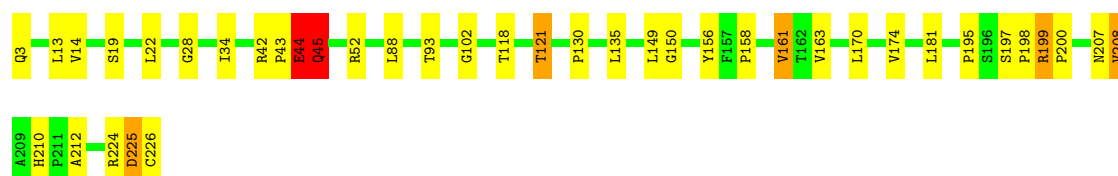
- Molecule 2: Antibody Heavy chain

Chain B: 



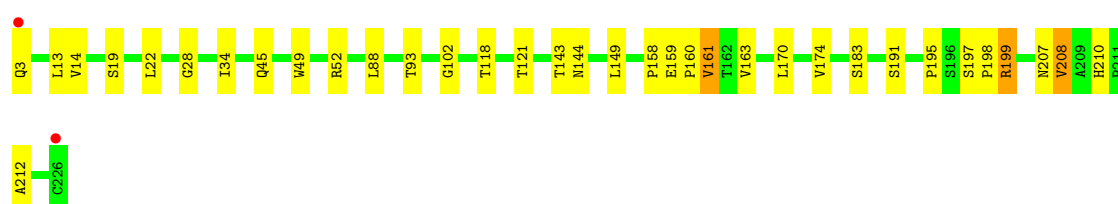
- Molecule 2: Antibody Heavy chain

Chain H: 



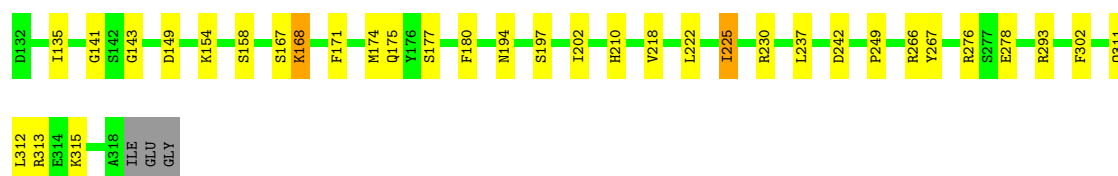
- Molecule 2: Antibody Heavy chain

Chain K: 



- Molecule 3: Integrin alpha-M

Chain G: 



- Molecule 3: Integrin alpha-M

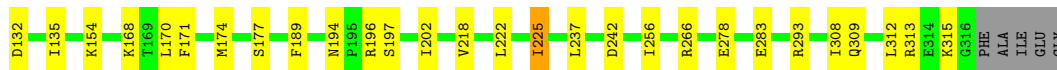
Chain E: 





• Molecule 3: Integrin alpha-M

Chain I:



• Molecule 3: Integrin alpha-M

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.60Å 158.35Å 233.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.00 47.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.65-3.00) 98.2 (47.65-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.194 , 0.224 0.202 , 0.230	Depositor DCC
R_{free} test set	3082 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61169 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, EDO

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	0/1757	0.68	0/2384
1	C	0.45	0/1757	0.67	0/2384
1	F	0.43	0/1757	0.69	0/2384
1	J	0.46	0/1757	0.71	0/2384
2	B	0.46	0/1732	0.74	0/2368
2	D	0.45	0/1732	0.76	0/2368
2	H	0.44	0/1732	0.75	2/2368 (0.1%)
2	K	0.46	0/1732	0.75	0/2368
3	E	0.46	0/1534	0.71	0/2063
3	G	0.46	0/1539	0.71	0/2070
3	I	0.45	0/1522	0.68	0/2047
3	L	0.46	0/1522	0.70	0/2047
All	All	0.45	0/20073	0.71	2/27235 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	44	GLU	C-N-CA	5.81	136.22	121.70
2	H	45	GLN	N-CA-C	5.17	124.96	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1647	16	0
1	C	1718	0	1647	19	0
1	F	1718	0	1647	15	0
1	J	1718	0	1647	13	0
2	B	1689	0	1638	19	0
2	D	1689	0	1638	22	0
2	H	1689	0	1638	20	0
2	K	1689	0	1638	18	0
3	E	1505	0	1515	14	0
3	G	1510	0	1520	18	0
3	I	1494	0	1506	13	0
3	L	1494	0	1506	7	0
4	C	8	0	12	0	0
4	D	8	0	12	6	0
4	H	4	0	6	0	0
4	J	8	0	12	0	0
4	K	4	0	6	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
5	G	12	0	16	5	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
7	A	2	0	0	0	0
7	B	8	0	0	0	0
7	C	9	0	0	1	0
7	D	5	0	0	0	0
7	E	6	0	0	1	0
7	F	8	0	0	0	0
7	G	4	0	0	0	0
7	H	6	0	0	0	0
7	I	3	0	0	0	0
7	J	9	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
All	All	19772	0	19275	190	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 5.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:199:ARG:HH11	2:K:199:ARG:HG3	1.09	1.17
2:B:199:ARG:HG3	2:B:199:ARG:HH11	1.19	1.03
2:H:199:ARG:HH11	2:H:199:ARG:HG3	1.18	1.03
2:D:199:ARG:HH11	2:D:199:ARG:HG3	1.30	0.95
2:K:199:ARG:CG	2:K:199:ARG:HH11	1.87	0.86
2:K:199:ARG:NH1	2:K:199:ARG:HG3	1.87	0.84
2:H:199:ARG:NH1	2:H:199:ARG:HG3	1.88	0.83
2:H:199:ARG:HD2	2:H:200:PRO:HA	1.65	0.79
2:D:199:ARG:HH11	2:D:199:ARG:CG	1.96	0.78
2:H:149:LEU:HD11	2:H:199:ARG:HG2	1.65	0.77
1:C:134:GLY:O	1:C:189:LYS:HB2	1.88	0.73
2:B:199:ARG:CG	2:B:199:ARG:HH11	1.99	0.73
3:L:218:VAL:HG11	3:L:237:LEU:HD13	1.73	0.70
3:E:218:VAL:HG11	3:E:237:LEU:HD13	1.73	0.70
1:F:201:GLU:HG3	1:F:212:VAL:HG22	1.74	0.70
3:I:218:VAL:HG11	3:I:237:LEU:HD13	1.74	0.69
1:C:37:ASN:HD21	1:C:74:GLY:H	1.40	0.69
1:F:37:ASN:HD21	1:F:74:GLY:H	1.41	0.68
3:L:162:GLU:HG2	3:L:195:PRO:HG2	1.75	0.68
2:B:199:ARG:HG3	2:B:199:ARG:NH1	1.99	0.68
3:G:218:VAL:HG11	3:G:237:LEU:HD13	1.76	0.68
1:A:37:ASN:HD21	1:A:74:GLY:H	1.41	0.68
1:J:37:ASN:HD21	1:J:74:GLY:H	1.41	0.66
3:G:180:PHE:O	5:G:6:GOL:H12	1.96	0.65
3:E:308:ILE:O	3:E:310:ASN:N	2.30	0.64
2:D:106:TYR:O	4:D:2:EDO:H22	1.96	0.64
3:G:249:PRO:HG3	5:G:5:GOL:H2	1.80	0.64
2:H:44:GLU:HA	2:H:45:GLN:O	1.97	0.63
2:D:199:ARG:NH1	2:D:199:ARG:HG3	2.08	0.63
2:K:34:ILE:HG22	2:K:102:GLY:HA2	1.82	0.61
3:E:304:ALA:O	3:E:307:THR:HB	2.01	0.61
2:D:103:HIS:HA	4:D:2:EDO:H21	1.83	0.60
2:D:34:ILE:HG22	2:D:102:GLY:HA2	1.85	0.59
1:C:37:ASN:ND2	1:C:74:GLY:H	2.00	0.59
1:J:37:ASN:ND2	1:J:74:GLY:H	2.01	0.59
1:C:187:LEU:HD13	1:C:192:TYR:HB2	1.84	0.58
1:A:37:ASN:ND2	1:A:74:GLY:H	2.01	0.58
3:L:279:LYS:O	3:L:282:GLN:HG2	2.03	0.58
1:F:37:ASN:ND2	1:F:74:GLY:H	2.01	0.58
1:F:188:THR:H	1:F:191:GLU:HB2	1.69	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:93:THR:HG23	2:D:121:THR:HA	1.87	0.57
2:B:149:LEU:HD11	2:B:199:ARG:HG2	1.85	0.57
2:H:42:ARG:O	2:H:44:GLU:N	2.39	0.56
3:I:194:ASN:HD22	3:I:197:SER:HB3	1.71	0.56
2:B:195:PRO:HB2	2:B:198:PRO:HD2	1.87	0.56
2:B:130:PRO:HB3	2:B:156:TYR:HB3	1.88	0.56
2:D:3:GLN:HE21	3:I:194:ASN:ND2	2.03	0.55
3:E:162:GLU:HG3	3:E:195:PRO:HG2	1.89	0.55
3:G:194:ASN:HD22	3:G:197:SER:HB3	1.72	0.54
1:F:201:GLU:HG2	1:F:210:PRO:HB2	1.89	0.54
3:E:194:ASN:HD22	3:E:197:SER:HB3	1.73	0.54
2:D:158:PRO:HD2	2:D:212:ALA:CB	2.37	0.54
2:K:199:ARG:CG	2:K:199:ARG:NH1	2.58	0.54
3:E:174:MET:HB2	3:E:222:LEU:HD11	1.90	0.54
3:I:174:MET:HB2	3:I:222:LEU:HD11	1.90	0.54
3:G:174:MET:HB2	3:G:222:LEU:HD11	1.90	0.53
2:D:103:HIS:HB3	4:D:2:EDO:H12	1.91	0.53
2:B:14:VAL:HG21	2:B:88:LEU:HD13	1.91	0.53
3:L:174:MET:HB2	3:L:222:LEU:HD11	1.90	0.52
1:A:196:ASN:HD21	1:A:218:ASN:HB2	1.73	0.52
1:J:156:ILE:HD11	1:J:185:LEU:HD21	1.91	0.52
1:F:31:TYR:CZ	1:F:33:SER:HB2	2.45	0.52
2:D:14:VAL:HG21	2:D:88:LEU:HD13	1.92	0.51
2:H:14:VAL:HG21	2:H:88:LEU:HD13	1.91	0.51
2:H:195:PRO:HB2	2:H:198:PRO:HD2	1.91	0.51
1:J:31:TYR:CZ	1:J:33:SER:HB2	2.46	0.51
2:D:195:PRO:O	2:D:198:PRO:HD2	2.09	0.51
2:D:195:PRO:HB2	2:D:198:PRO:HD2	1.92	0.51
2:K:22:LEU:HD22	2:K:118:THR:HG21	1.92	0.51
1:C:31:TYR:CZ	1:C:33:SER:HB2	2.46	0.51
1:A:31:TYR:CZ	1:A:33:SER:HB2	2.46	0.50
2:K:149:LEU:HD11	2:K:199:ARG:HG2	1.92	0.50
4:D:2:EDO:H11	3:G:143:GLY:CA	2.41	0.50
2:D:22:LEU:HD22	2:D:118:THR:HG21	1.94	0.50
2:B:199:ARG:HD2	2:B:200:PRO:HA	1.93	0.50
2:H:34:ILE:HG22	2:H:102:GLY:HA2	1.93	0.50
2:K:14:VAL:HG21	2:K:88:LEU:HD13	1.94	0.50
2:H:22:LEU:HD22	2:H:118:THR:HG21	1.94	0.49
2:K:93:THR:HG23	2:K:121:THR:HA	1.93	0.49
2:D:199:ARG:NH1	2:D:199:ARG:CG	2.65	0.49
3:G:210:HIS:CE1	5:G:5:GOL:H31	2.48	0.49
1:C:21:MET:HG2	1:C:108:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:MET:HG2	1:A:108:THR:HG21	1.95	0.49
3:G:210:HIS:HE1	5:G:5:GOL:H31	1.78	0.48
1:C:21:MET:HB3	7:C:223:HOH:O	2.12	0.48
3:G:249:PRO:CG	5:G:5:GOL:H2	2.43	0.48
1:F:21:MET:HG2	1:F:108:THR:HG21	1.96	0.48
2:B:22:LEU:HD22	2:B:118:THR:HG21	1.95	0.48
3:G:267:TYR:CE2	3:G:315:LYS:HG2	2.49	0.47
3:I:170:LEU:HD23	3:I:189:PHE:HD2	1.79	0.47
2:B:13:LEU:HD21	2:B:158:PRO:HB3	1.95	0.47
1:J:67:ARG:HG3	1:J:81:ILE:HG23	1.96	0.47
1:A:67:ARG:HG3	1:A:81:ILE:HG23	1.96	0.47
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.97	0.47
2:B:181:LEU:HB2	2:B:186:TYR:CE1	2.50	0.47
1:J:100:TYR:HD1	2:K:49:TRP:CH2	2.32	0.47
2:B:34:ILE:HG22	2:B:102:GLY:HA2	1.96	0.47
1:A:166:LEU:HD21	2:B:182:GLN:HG3	1.96	0.47
2:B:195:PRO:O	2:B:198:PRO:HD2	2.15	0.46
2:H:158:PRO:HD2	2:H:212:ALA:CB	2.45	0.46
1:F:67:ARG:HG3	1:F:81:ILE:HG23	1.97	0.46
3:E:236:ILE:HG21	3:E:317:PHE:HB3	1.97	0.46
1:J:21:MET:HG2	1:J:108:THR:HG21	1.97	0.46
2:K:195:PRO:HB2	2:K:198:PRO:HD2	1.97	0.46
3:E:166:LYS:O	3:E:168:LYS:N	2.49	0.45
2:B:35:TYR:HB2	2:B:101:GLU:HB3	1.97	0.45
3:I:256:ILE:HG23	3:I:266:ARG:HH21	1.80	0.45
1:C:67:ARG:HG3	1:C:81:ILE:HG23	1.97	0.45
2:K:195:PRO:O	2:K:198:PRO:HD2	2.16	0.45
2:D:163:VAL:HG22	2:D:208:VAL:HB	1.99	0.45
2:K:161:VAL:HG23	2:K:210:HIS:HD2	1.82	0.45
1:C:89:LEU:HD11	1:C:112:LEU:HD13	1.98	0.45
3:G:135:ILE:O	3:G:171:PHE:HA	2.17	0.44
2:H:225:ASP:HB3	2:H:226:CYS:HB3	2.00	0.44
2:D:195:PRO:C	2:D:198:PRO:HD2	2.38	0.44
1:A:89:LEU:HD11	1:A:112:LEU:HD13	2.00	0.44
4:D:2:EDO:H11	3:G:143:GLY:HA2	1.99	0.44
1:F:89:LEU:HD11	1:F:112:LEU:HD13	1.99	0.44
2:H:163:VAL:HG22	2:H:208:VAL:HB	2.00	0.44
2:H:93:THR:HG23	2:H:121:THR:HA	2.00	0.44
2:K:13:LEU:HD12	2:K:121:THR:HB	2.00	0.43
1:A:138:VAL:HG13	1:A:185:LEU:HB3	1.99	0.43
2:D:149:LEU:HD11	2:D:199:ARG:HG2	2.00	0.43
3:I:132:ASP:N	3:I:168:LYS:HB3	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:93:THR:HG23	2:B:121:THR:HA	1.99	0.43
3:I:170:LEU:CD2	3:I:189:PHE:HD2	2.31	0.43
1:F:114:ARG:HD3	1:F:115:ALA:O	2.17	0.43
1:C:138:VAL:HG13	1:C:185:LEU:HB3	2.00	0.43
1:J:89:LEU:HD11	1:J:112:LEU:HD13	2.00	0.43
4:D:2:EDO:H11	3:G:143:GLY:HA3	2.00	0.43
3:E:225:ILE:HG13	3:E:225:ILE:H	1.64	0.43
1:A:17:GLU:O	1:A:84:VAL:HG23	2.19	0.43
2:B:195:PRO:HB2	2:B:198:PRO:CD	2.48	0.43
1:F:125:PRO:HB2	2:H:224:ARG:NH2	2.34	0.43
1:C:156:ILE:HD11	1:C:185:LEU:HD21	2.00	0.43
2:H:161:VAL:HG23	2:H:210:HIS:HD2	1.83	0.43
1:J:17:GLU:O	1:J:84:VAL:HG23	2.19	0.43
2:B:163:VAL:HG22	2:B:208:VAL:HB	2.01	0.43
1:A:199:THR:HG23	1:A:214:SER:HB2	2.00	0.43
1:C:199:THR:HG23	1:C:214:SER:HB2	2.00	0.42
2:D:195:PRO:HD2	2:D:198:PRO:HG3	2.01	0.42
1:A:114:ARG:HD3	1:A:115:ALA:O	2.19	0.42
3:L:154:LYS:HD3	3:L:202:ILE:HB	2.01	0.42
1:C:201:GLU:HG2	1:C:212:VAL:HG22	2.01	0.42
2:K:158:PRO:HD2	2:K:212:ALA:CB	2.49	0.42
1:J:114:ARG:HD3	1:J:115:ALA:O	2.19	0.42
2:D:195:PRO:HB2	2:D:198:PRO:CD	2.50	0.42
1:F:17:GLU:O	1:F:84:VAL:HG23	2.19	0.42
1:C:139:VAL:HG22	1:C:184:THR:HG23	2.02	0.42
2:K:163:VAL:HG22	2:K:208:VAL:HB	2.02	0.42
1:C:114:ARG:HD3	1:C:115:ALA:O	2.20	0.42
1:J:199:THR:HG23	1:J:214:SER:HB2	2.01	0.42
1:F:199:THR:HG23	1:F:214:SER:HB2	2.01	0.42
3:I:312:LEU:HG	3:I:313:ARG:H	1.85	0.42
1:F:167:ASN:ND2	1:F:183:SER:OG	2.52	0.41
2:H:44:GLU:HA	2:H:45:GLN:C	2.41	0.41
1:C:17:GLU:O	1:C:84:VAL:HG23	2.20	0.41
3:E:135:ILE:O	3:E:171:PHE:HA	2.21	0.41
3:E:280:SER:O	3:E:283:GLU:HB3	2.21	0.41
3:L:271:VAL:HG13	3:L:299:VAL:HG23	2.03	0.41
3:I:170:LEU:HD23	3:I:189:PHE:CD2	2.56	0.41
2:K:159:GLU:HG3	2:K:160:PRO:HA	2.03	0.41
3:G:154:LYS:HD3	3:G:202:ILE:HB	2.02	0.41
3:L:225:ILE:HG13	3:L:225:ILE:H	1.64	0.41
2:B:195:PRO:C	2:B:198:PRO:HD2	2.41	0.41
2:K:210:HIS:CE1	2:K:212:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:195:PRO:O	2:H:198:PRO:HD2	2.20	0.41
1:C:153:LYS:HB2	1:C:201:GLU:HB2	2.03	0.41
1:A:13:VAL:HG22	1:A:19:VAL:HG11	2.03	0.41
1:A:201:GLU:HG2	1:A:212:VAL:HG22	2.02	0.41
2:D:49:TRP:CZ2	2:D:51:GLY:HA2	2.56	0.41
3:E:245:LYS:NZ	7:E:39:HOH:O	2.49	0.41
3:G:149:ASP:HB3	3:G:302:PHE:CD2	2.56	0.41
2:H:135:LEU:HB2	2:H:150:GLY:CA	2.51	0.41
3:G:168:LYS:HG3	3:G:230:ARG:NH2	2.36	0.41
1:C:189:LYS:O	1:C:193:GLU:HG3	2.21	0.40
3:E:154:LYS:HD3	3:E:202:ILE:HB	2.03	0.40
3:I:225:ILE:H	3:I:225:ILE:HG13	1.63	0.40
1:J:97:TYR:HA	1:J:102:LEU:HD22	2.03	0.40
1:F:75:THR:HG22	1:F:76:ASP:OD1	2.22	0.40
2:D:130:PRO:HB3	2:D:156:TYR:HB3	2.04	0.40
3:G:225:ILE:HG13	3:G:225:ILE:H	1.65	0.40
3:G:141:GLY:HA3	3:G:175:GLN:OE1	2.21	0.40
3:I:154:LYS:HD3	3:I:202:ILE:HB	2.02	0.40
1:C:13:VAL:HG22	1:C:19:VAL:HG11	2.03	0.40
1:J:13:VAL:HG11	1:J:84:VAL:HG11	2.04	0.40
1:A:97:TYR:HA	1:A:102:LEU:HD22	2.04	0.40
3:E:141:GLY:HA3	3:E:175:GLN:OE1	2.21	0.40
1:A:75:THR:HG22	1:A:76:ASP:OD1	2.22	0.40
3:I:135:ILE:O	3:I:171:PHE:HA	2.21	0.40

There are no symmetry-related clashes.

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	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
1	C	218/220 (99%)	209 (96%)	8 (4%)	1 (0%)	38	84
1	F	218/220 (99%)	208 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	218/220 (99%)	208 (95%)	9 (4%)	1 (0%)	38	84
2	B	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	13	53
2	D	222/224 (99%)	213 (96%)	5 (2%)	4 (2%)	13	53
2	H	222/224 (99%)	213 (96%)	5 (2%)	4 (2%)	13	53
2	K	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	16	60
3	E	184/190 (97%)	170 (92%)	10 (5%)	4 (2%)	10	45
3	G	185/190 (97%)	172 (93%)	11 (6%)	2 (1%)	21	67
3	I	183/190 (96%)	173 (94%)	9 (5%)	1 (0%)	38	84
3	L	183/190 (96%)	173 (94%)	8 (4%)	2 (1%)	21	67
All	All	2495/2536 (98%)	2366 (95%)	103 (4%)	26 (1%)	22	70

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	43	PRO
2	B	225	ASP
3	E	167	SER
3	E	309	GLN
2	H	45	GLN
2	B	143	THR
3	E	308	ILE
2	H	43	PRO
2	D	183	SER
2	D	225	ASP
2	H	44	GLU
2	K	143	THR
3	L	315	LYS
3	G	167	SER
3	G	177	SER
1	J	163	ASN
3	E	177	SER
3	I	177	SER
2	K	183	SER
3	L	177	SER
1	C	135	GLY
2	D	28	GLY
2	B	28	GLY
2	H	28	GLY
2	K	28	GLY

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Mol	Chain	Res	Type
2	B	4	VAL

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	197/197 (100%)	181 (92%)	16 (8%)	17	53
1	C	197/197 (100%)	179 (91%)	18 (9%)	14	46
1	F	197/197 (100%)	180 (91%)	17 (9%)	15	50
1	J	197/197 (100%)	181 (92%)	16 (8%)	17	53
2	B	192/192 (100%)	176 (92%)	16 (8%)	16	52
2	D	192/192 (100%)	176 (92%)	16 (8%)	16	52
2	H	192/192 (100%)	178 (93%)	14 (7%)	20	59
2	K	192/192 (100%)	179 (93%)	13 (7%)	22	63
3	E	166/168 (99%)	153 (92%)	13 (8%)	18	55
3	G	166/168 (99%)	155 (93%)	11 (7%)	24	64
3	I	165/168 (98%)	156 (94%)	9 (6%)	30	73
3	L	165/168 (98%)	152 (92%)	13 (8%)	18	54
All	All	2218/2228 (100%)	2046 (92%)	172 (8%)	18	55

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	THR
1	C	7	SER
1	C	10	SER
1	C	27	GLN
1	C	39	LEU
1	C	51	LYS
1	C	95	GLN
1	C	111	GLU
1	C	114	ARG
1	C	123	ILE

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Mol	Chain	Res	Type
1	C	160	GLU
1	C	162	GLN
1	C	166	LEU
1	C	182	SER
1	C	187	LEU
1	C	195	HIS
1	C	197	SER
1	C	203	THR
2	D	19	SER
2	D	45	GLN
2	D	52	ARG
2	D	91	GLU
2	D	119	THR
2	D	143	THR
2	D	161	VAL
2	D	170	LEU
2	D	174	VAL
2	D	184	ASP
2	D	185	LEU
2	D	189	SER
2	D	197	SER
2	D	199	ARG
2	D	207	ASN
2	D	208	VAL
3	G	158	SER
3	G	168	LYS
3	G	225	ILE
3	G	242	ASP
3	G	266	ARG
3	G	276	ARG
3	G	278	GLU
3	G	293	ARG
3	G	311	GLN
3	G	312	LEU
3	G	313	ARG
1	A	3	GLU
1	A	5	THR
1	A	7	SER
1	A	10	SER
1	A	27	GLN
1	A	39	LEU
1	A	51	LYS

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	111	GLU
1	A	114	ARG
1	A	123	ILE
1	A	138	VAL
1	A	166	LEU
1	A	182	SER
1	A	197	SER
1	A	203	THR
2	B	19	SER
2	B	44	GLU
2	B	45	GLN
2	B	52	ARG
2	B	91	GLU
2	B	142	GLN
2	B	145	SER
2	B	161	VAL
2	B	170	LEU
2	B	174	VAL
2	B	182	GLN
2	B	197	SER
2	B	199	ARG
2	B	207	ASN
2	B	208	VAL
2	B	226	CYS
3	E	164	LEU
3	E	166	LYS
3	E	168	LYS
3	E	225	ILE
3	E	226	THR
3	E	242	ASP
3	E	278	GLU
3	E	281	ARG
3	E	293	ARG
3	E	307	THR
3	E	312	LEU
3	E	313	ARG
3	E	315	LYS
1	F	5	THR
1	F	7	SER
1	F	10	SER
1	F	27	GLN

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Mol	Chain	Res	Type
1	F	39	LEU
1	F	51	LYS
1	F	95	GLN
1	F	111	GLU
1	F	114	ARG
1	F	166	LEU
1	F	182	SER
1	F	187	LEU
1	F	190	ASP
1	F	197	SER
1	F	203	THR
1	F	218	ASN
1	F	220	CYS
2	H	3	GLN
2	H	13	LEU
2	H	19	SER
2	H	52	ARG
2	H	121	THR
2	H	161	VAL
2	H	170	LEU
2	H	174	VAL
2	H	181	LEU
2	H	197	SER
2	H	199	ARG
2	H	207	ASN
2	H	208	VAL
2	H	225	ASP
3	I	196	ARG
3	I	225	ILE
3	I	242	ASP
3	I	278	GLU
3	I	283	GLU
3	I	293	ARG
3	I	308	ILE
3	I	309	GLN
3	I	315	LYS
1	J	5	THR
1	J	7	SER
1	J	10	SER
1	J	27	GLN
1	J	39	LEU
1	J	51	LYS

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Mol	Chain	Res	Type
1	J	95	GLN
1	J	111	GLU
1	J	114	ARG
1	J	138	VAL
1	J	161	ARG
1	J	166	LEU
1	J	182	SER
1	J	187	LEU
1	J	203	THR
1	J	218	ASN
2	K	3	GLN
2	K	19	SER
2	K	45	GLN
2	K	52	ARG
2	K	144	ASN
2	K	161	VAL
2	K	170	LEU
2	K	174	VAL
2	K	191	SER
2	K	197	SER
2	K	199	ARG
2	K	207	ASN
2	K	208	VAL
3	L	151	ARG
3	L	155	GLU
3	L	158	SER
3	L	225	ILE
3	L	242	ASP
3	L	273	ASP
3	L	279	LYS
3	L	283	GLU
3	L	293	ARG
3	L	300	ASN
3	L	307	THR
3	L	311	GLN
3	L	314	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	ASN
1	C	95	GLN

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Mol	Chain	Res	Type
1	C	167	ASN
1	C	216	ASN
2	D	7	GLN
2	D	30	ASN
3	G	194	ASN
3	G	311	GLN
1	A	37	ASN
1	A	95	GLN
1	A	167	ASN
1	A	196	ASN
1	A	216	ASN
1	A	218	ASN
2	B	7	GLN
2	B	30	ASN
2	B	45	GLN
2	B	142	GLN
3	E	194	ASN
3	E	285	ASN
1	F	37	ASN
1	F	95	GLN
1	F	167	ASN
2	H	30	ASN
2	H	45	GLN
2	H	182	GLN
3	I	194	ASN
3	I	309	GLN
1	J	37	ASN
1	J	95	GLN
1	J	167	ASN
2	K	30	ASN
3	L	282	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	221	-	5,5,5	0.74	0	5,5,5	1.05	0
5	GOL	B	1	-	5,5,5	0.78	0	5,5,5	0.95	0
4	EDO	C	221	-	3,3,3	0.62	0	2,2,2	0.06	0
4	EDO	C	222	-	3,3,3	0.56	0	2,2,2	0.45	0
4	EDO	D	2	-	3,3,3	0.68	0	2,2,2	0.06	0
5	GOL	D	227	-	5,5,5	1.00	0	5,5,5	0.83	0
4	EDO	D	228	-	3,3,3	0.64	0	2,2,2	0.21	0
5	GOL	G	5	-	5,5,5	0.74	0	5,5,5	1.10	0
5	GOL	G	6	-	5,5,5	0.86	0	5,5,5	0.96	0
4	EDO	H	227	-	3,3,3	0.63	0	2,2,2	0.24	0
4	EDO	J	221	-	3,3,3	0.69	0	2,2,2	0.12	0
4	EDO	J	222	-	3,3,3	0.69	0	2,2,2	0.09	0
4	EDO	K	227	-	3,3,3	0.59	0	2,2,2	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	221	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1	-	-	0/4/4/4	0/0/0/0
4	EDO	C	221	-	-	0/1/1/1	0/0/0/0
4	EDO	C	222	-	-	0/1/1/1	0/0/0/0
4	EDO	D	2	-	-	0/1/1/1	0/0/0/0
5	GOL	D	227	-	-	0/4/4/4	0/0/0/0
4	EDO	D	228	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	G	5	-	-	0/4/4/4	0/0/0/0
5	GOL	G	6	-	-	0/4/4/4	0/0/0/0
4	EDO	H	227	-	-	0/1/1/1	0/0/0/0
4	EDO	J	221	-	-	0/1/1/1	0/0/0/0
4	EDO	J	222	-	-	0/1/1/1	0/0/0/0
4	EDO	K	227	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	220/220 (100%)	-0.19	0	100 100	32, 55, 88, 111	0
1	C	220/220 (100%)	-0.27	0	100 100	22, 39, 78, 110	0
1	F	220/220 (100%)	-0.29	0	100 100	23, 43, 66, 111	0
1	J	220/220 (100%)	-0.30	1 (0%)	88 36	24, 43, 63, 109	0
2	B	224/224 (100%)	-0.31	1 (0%)	90 41	21, 39, 77, 104	0
2	D	224/224 (100%)	-0.30	0	100 100	19, 36, 68, 106	0
2	H	224/224 (100%)	-0.22	0	100 100	21, 44, 77, 105	0
2	K	224/224 (100%)	-0.27	2 (0%)	81 24	23, 41, 75, 104	0
3	E	186/190 (97%)	-0.23	0	100 100	27, 53, 86, 99	0
3	G	187/190 (98%)	-0.27	0	100 100	24, 42, 77, 100	0
3	I	185/190 (97%)	0.06	0	100 100	39, 79, 113, 126	0
3	L	185/190 (97%)	-0.24	0	100 100	28, 51, 85, 102	0
All	All	2519/2536 (99%)	-0.24	4 (0%)	93 54	19, 44, 87, 126	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	226	CYS	3.0
2	K	3	GLN	2.5
1	J	220	CYS	2.4
2	B	3	GLN	2.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	C	221	4/4	0.39	9.57	51,51,51,57	0
4	EDO	K	227	4/4	0.44	9.43	53,55,56,57	0
5	GOL	G	5	6/6	0.38	7.03	60,61,61,62	0
4	EDO	J	221	4/4	0.43	6.95	42,43,45,46	0
4	EDO	D	2	4/4	0.33	6.17	49,50,51,54	0
5	GOL	B	1	6/6	0.32	4.98	52,54,54,55	0
5	GOL	G	6	6/6	0.29	4.17	55,56,56,56	0
4	EDO	J	222	4/4	0.32	3.91	48,49,49,53	0
5	GOL	D	227	6/6	0.28	3.53	58,59,59,59	0
4	EDO	H	227	4/4	0.19	1.02	53,55,56,56	0
4	EDO	C	222	4/4	0.19	0.30	51,53,56,66	0
5	GOL	A	221	6/6	0.23	-0.12	60,61,61,61	0
4	EDO	D	228	4/4	0.16	-0.16	64,65,65,70	0
6	CA	I	500	1/1	0.15	-1.19	49,49,49,49	0
6	CA	L	500	1/1	0.15	-1.79	49,49,49,49	0
6	CA	G	500	1/1	0.14	-2.41	28,28,28,28	0
6	CA	E	500	1/1	0.11	-2.70	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.