Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 12:03 pm BST

PDB ID	:	7A4D
Title	:	Crystal structure of the APH coiled-coil in complex with nanobodies Nb28 and Nb30
Authors	:	Hadzi, S.
Deposited on	:	2020-08-19
Resolution	:	2.69 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:

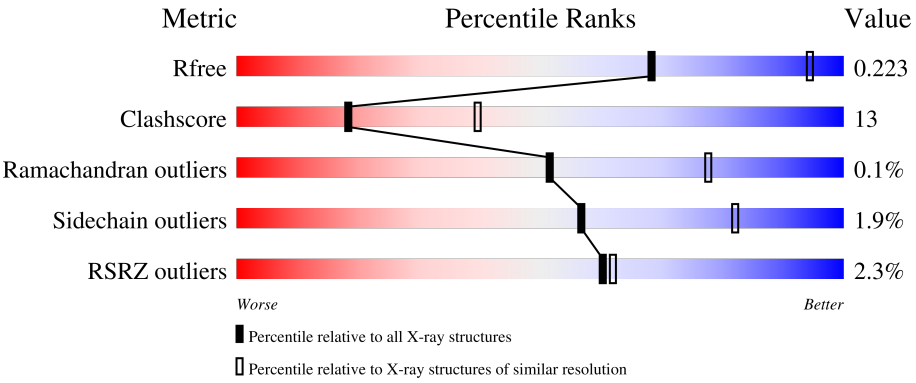
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	133	73% 13% • 11%
1	B	133	3% 68% 20% • 12%
1	G	133	71% 19% • 10%
1	H	133	77% 9% • 13%
2	C	130	4% 68% 17% • 13%

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Mol	Chain	Length	Quality of chain
2	D	130	2% 65% 18% 14%
2	I	130	4% 72% 14% 13%
2	J	130	5% 62% 25% 13%
3	E	42	81% 19%
3	F	42	76% 19%
3	K	42	2% 74% 21% 5%
3	L	42	64% 26% 5% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8422 atoms, of which 29 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 Nanobody Nb28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			889	554	153	177	5			
1	B	117	Total	C	N	O	S	0	0	0
			885	552	152	176	5			
1	G	120	Total	C	N	O	S	0	0	0
			897	559	154	179	5			
1	H	116	Total	C	N	O	S	0	0	0
			880	549	151	175	5			

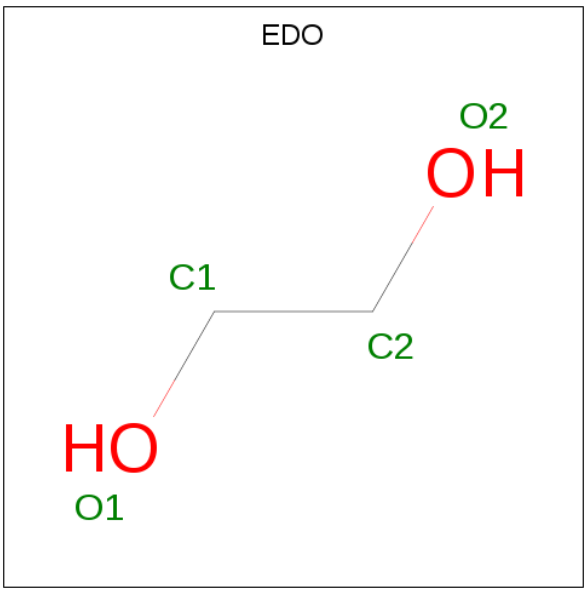
- Molecule 2 is a protein called Nanobody Nb30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	S	0	0	0
			862	537	153	168	4			
2	D	112	Total	C	N	O	S	0	0	0
			855	533	150	168	4			
2	I	113	Total	C	N	O	S	0	1	0
			865	542	150	169	4			
2	J	113	Total	C	N	O	S	0	0	0
			851	531	149	167	4			

- Molecule 3 is a protein called APH coiled-coil.

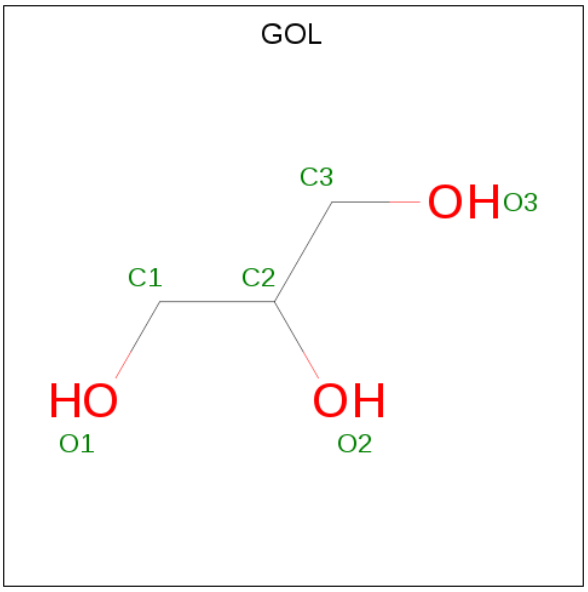
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	42	Total	C	N	O	0	0	1
			338	212	58	68			
3	F	41	Total	C	N	O	0	0	0
			326	204	56	66			
3	K	40	Total	C	N	O	0	0	0
			327	204	56	67			
3	L	40	Total	C	N	O	0	0	0
			337	213	57	67			

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



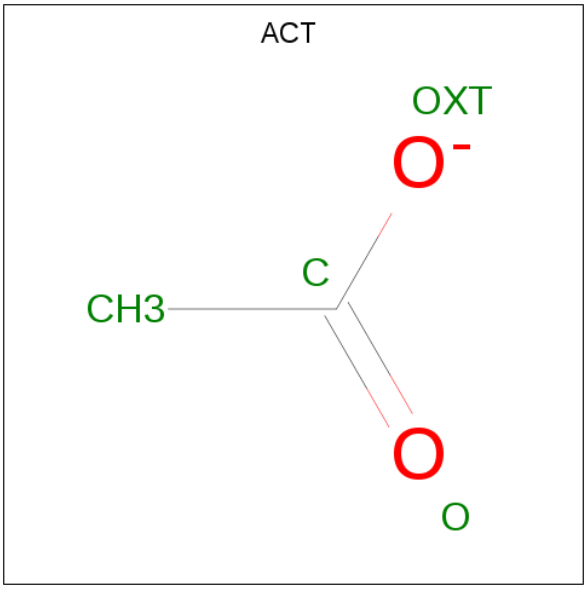
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	4	Total	O	0	0
			4	4		
7	C	8	Total	O	0	0
			8	8		
7	D	9	Total	O	0	0
			9	9		
7	E	1	Total	O	0	0
			1	1		
7	F	2	Total	O	0	0
			2	2		
7	G	5	Total	O	0	0
			5	5		
7	H	15	Total	O	0	0
			15	15		

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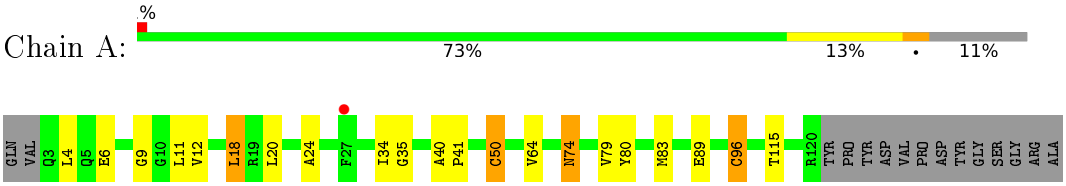
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	4	Total O 4 4	0	0
7	J	3	Total O 3 3	0	0
7	K	1	Total O 1 1	0	0
7	L	1	Total O 1 1	0	0

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.

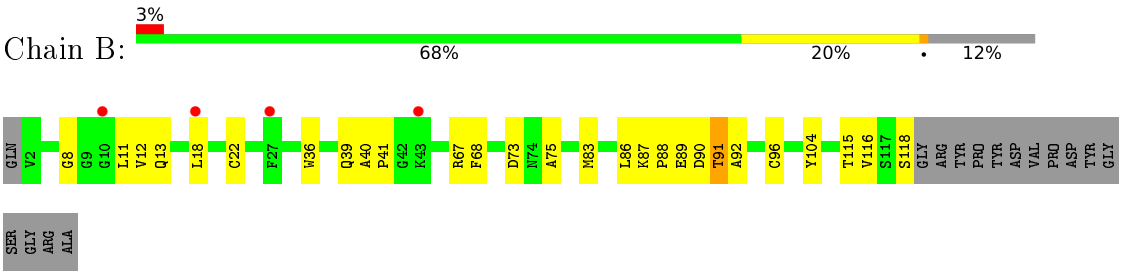
- Molecule 1: Nanobody Nb28

Chain A:



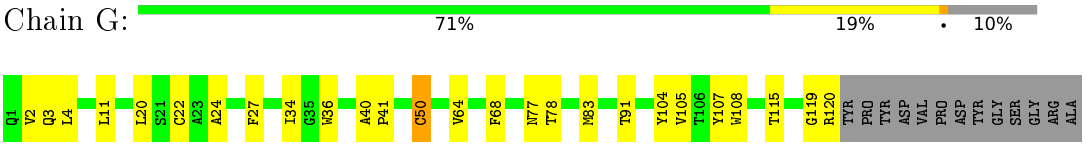
- Molecule 1: Nanobody Nb28

Chain B:



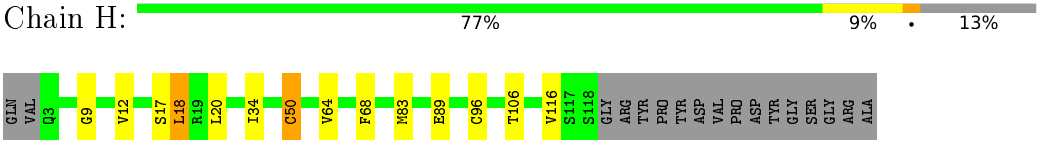
- Molecule 1: Nanobody Nb28

Chain G:



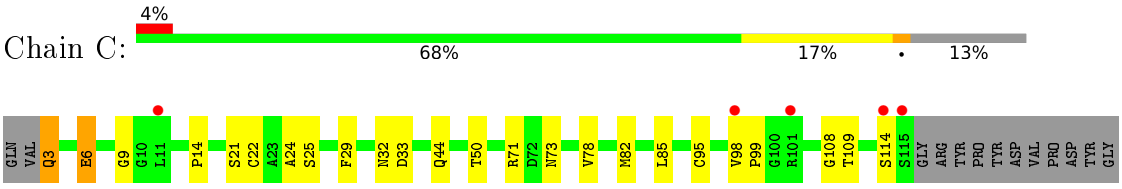
- Molecule 1: Nanobody Nb28

Chain H:



- Molecule 2: Nanobody Nb30

Chain C:

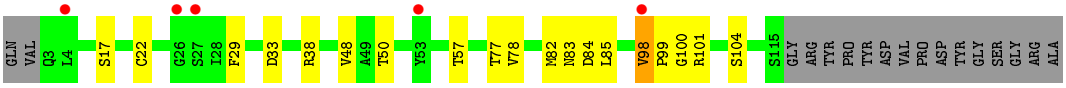


• Molecule 2: Nanobody Nb30

Chain D:

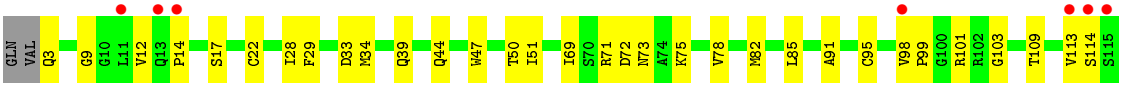
• Molecule 2: Nanobody Nb30

Chain I:



• Molecule 2: Nanobody Nb30

Chain J:

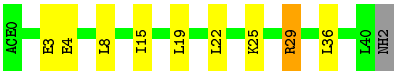


• Molecule 3: APH coiled-coil

Chain E:

• Molecule 3: APH coiled-coil

Chain F:



• Molecule 3: APH coiled-coil

Chain K:

• Molecule 3: APH coiled-coil

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.26Å 127.45Å 192.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.69 48.23 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.23-2.69) 99.4 (48.23-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.176 , 0.223 0.180 , 0.223	Depositor DCC
R_{free} test set	2121 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8422	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, NH2, EDO, ACE

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	0.97	5/908 (0.6%)	0.76	1/1231 (0.1%)
1	B	1.02	1/904 (0.1%)	0.76	0/1226
1	G	0.51	1/916 (0.1%)	0.68	0/1244
1	H	0.66	2/899 (0.2%)	0.72	1/1219 (0.1%)
2	C	0.51	0/883	0.69	0/1201
2	D	0.57	1/876 (0.1%)	0.75	2/1192 (0.2%)
2	I	0.49	0/890	0.68	0/1212
2	J	0.42	0/872	0.64	0/1189
3	E	0.60	0/336	0.61	0/447
3	F	0.40	0/325	0.61	0/434
3	K	0.58	0/328	0.65	0/437
3	L	0.47	0/338	0.68	1/449 (0.2%)
All	All	0.66	10/8475 (0.1%)	0.70	5/11481 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	96	CYS	CB-SG	-9.16	1.66	1.82
1	A	96	CYS	CB-SG	-8.60	1.67	1.82
1	A	50	CYS	CB-SG	-7.19	1.70	1.82
1	H	50	CYS	CB-SG	-6.47	1.71	1.82
1	A	80	TYR	CE1-CZ	-5.43	1.31	1.38
2	D	95	CYS	CB-SG	-5.33	1.73	1.81
1	B	96	CYS	CB-SG	-5.32	1.73	1.81
1	G	50	CYS	CB-SG	-5.18	1.73	1.81
1	A	80	TYR	CG-CD1	-5.13	1.32	1.39
1	A	80	TYR	CE2-CZ	-5.12	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	98	VAL	N-CA-C	6.28	127.96	111.00
2	D	99	PRO	N-CA-C	-6.06	96.34	112.10
1	H	18	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	18	LEU	CA-CB-CG	5.69	128.38	115.30
3	L	36	LEU	CA-CB-CG	-5.03	103.73	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	889	0	841	20	0
1	B	885	0	838	22	0
1	G	897	0	844	19	0
1	H	880	0	836	14	0
2	C	862	0	805	29	0
2	D	855	0	798	24	0
2	I	865	0	803	20	0
2	J	851	0	780	44	0
3	E	338	0	346	15	0
3	F	326	0	322	12	0
3	K	327	0	325	13	0
3	L	337	0	354	17	0
4	A	4	6	6	0	0
4	B	4	6	6	0	0
4	H	4	6	6	0	0
5	D	6	8	8	0	0
6	G	4	3	3	0	0
7	A	6	0	0	0	0
7	B	4	0	0	0	0
7	C	8	0	0	0	0
7	D	9	0	0	0	0
7	E	1	0	0	0	0
7	F	2	0	0	0	0
7	G	5	0	0	0	0
7	H	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	4	0	0	0	0
7	J	3	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
All	All	8393	29	7921	216	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 13.

All (216) 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:J:51:ILE:HD11	2:J:69:ILE:HG12	1.16	1.11
2:J:98:VAL:CG1	2:J:99:PRO:HD3	1.90	1.00
2:J:51:ILE:CD1	2:J:69:ILE:HG12	1.94	0.97
2:J:98:VAL:HG13	2:J:99:PRO:HD3	1.47	0.96
2:C:98:VAL:HG11	3:E:29:ARG:NH2	1.84	0.92
2:I:50:THR:HG23	2:I:98:VAL:HG11	1.50	0.92
2:D:98:VAL:HG12	2:D:99:PRO:HD3	1.55	0.87
2:D:40:PRO:HB2	2:D:43:LYS:HD2	1.58	0.85
2:C:50:THR:HG23	2:C:98:VAL:HG21	1.60	0.83
2:J:44:GLN:NE2	3:K:3:GLU:HA	1.94	0.83
2:J:33:ASP:HB2	2:J:98:VAL:CG1	2.09	0.82
2:C:98:VAL:HG11	3:E:29:ARG:HH21	1.41	0.82
2:J:9:GLY:H	2:J:109:THR:HG21	1.45	0.81
1:A:20:LEU:HG	1:A:83:MET:HE2	1.64	0.78
2:C:22:CYS:HB3	2:C:78:VAL:HG12	1.64	0.77
1:B:88:PRO:HA	1:B:116:VAL:HG13	1.66	0.77
2:J:44:GLN:HE21	3:K:3:GLU:HA	1.49	0.76
2:J:98:VAL:HG12	2:J:99:PRO:HD3	1.66	0.75
2:C:98:VAL:HG12	2:C:99:PRO:HD3	1.69	0.75
1:G:40:ALA:HB1	1:G:41:PRO:HD2	1.68	0.74
2:D:9:GLY:H	2:D:109:THR:HG21	1.52	0.73
2:J:33:ASP:HB2	2:J:98:VAL:HG11	1.70	0.73
2:C:22:CYS:HB3	2:C:78:VAL:CG1	2.18	0.72
2:D:3:GLN:N	2:D:3:GLN:OE1	2.23	0.71
3:E:11:GLU:OE2	3:F:29:ARG:NH1	2.24	0.70
3:E:5:LEU:HD12	3:F:36:LEU:HD23	1.74	0.70
1:B:68:PHE:CZ	1:B:83:MET:HG2	2.27	0.69
3:L:1:LEU:HD13	3:L:2:GLU:H	1.58	0.69
3:L:1:LEU:CD1	3:L:2:GLU:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:THR:CG2	2:C:98:VAL:HG21	2.23	0.68
1:H:89:GLU:OE2	1:H:89:GLU:N	2.26	0.68
1:B:40:ALA:HB1	1:B:41:PRO:HD2	1.74	0.68
2:D:98:VAL:CG1	2:D:99:PRO:HD3	2.24	0.68
2:C:3:GLN:CG	2:C:25:SER:HB2	2.23	0.68
2:I:33:ASP:CB	2:I:98:VAL:HG12	2.24	0.67
3:K:22:LEU:HD22	3:L:15:ILE:HG23	1.77	0.67
2:J:29:PHE:HA	2:J:34:MET:HE3	1.77	0.66
2:C:3:GLN:HG3	2:C:25:SER:HB2	1.80	0.64
1:A:74:ASN:H	1:A:74:ASN:ND2	1.95	0.64
2:J:98:VAL:HG13	2:J:99:PRO:CD	2.25	0.64
2:I:33:ASP:HB2	2:I:98:VAL:HG12	1.79	0.63
1:G:64:VAL:HG13	1:G:68:PHE:CG	2.32	0.63
1:A:34:ILE:O	1:A:50:CYS:HB2	1.99	0.63
1:A:9:GLY:HA2	1:A:18:LEU:HD22	1.80	0.62
1:B:91:THR:OG1	1:B:116:VAL:HG12	2.01	0.61
2:J:51:ILE:HG12	2:J:69:ILE:CG2	2.30	0.61
2:I:82:MET:HE2	2:I:85:LEU:HD21	1.82	0.60
2:D:98:VAL:HG22	2:D:98:VAL:O	2.00	0.60
2:C:98:VAL:HG12	2:C:99:PRO:CD	2.32	0.60
2:C:50:THR:HG23	2:C:98:VAL:CG2	2.30	0.60
2:J:51:ILE:CG1	2:J:69:ILE:HG12	2.31	0.59
3:K:19:LEU:HD21	3:L:22:LEU:HB3	1.83	0.59
1:H:20:LEU:HG	1:H:83:MET:HE2	1.84	0.59
2:I:50:THR:CG2	2:I:98:VAL:HG11	2.30	0.59
2:J:51:ILE:HG12	2:J:69:ILE:HG23	1.84	0.59
1:A:35:GLY:HA2	1:A:50:CYS:CB	2.32	0.59
1:H:9:GLY:HA2	1:H:18:LEU:CD2	2.33	0.59
1:B:11:LEU:HD12	1:B:115:THR:O	2.03	0.58
1:G:20:LEU:HG	1:G:83:MET:HE2	1.85	0.58
3:L:1:LEU:HD13	3:L:2:GLU:N	2.18	0.58
1:A:6:GLU:HG3	1:A:96:CYS:HB2	1.84	0.58
2:C:6:GLU:N	2:C:6:GLU:OE2	2.37	0.58
3:E:22:LEU:HD22	3:F:15:ILE:HG23	1.86	0.58
1:B:87:LYS:HB3	1:B:88:PRO:HD2	1.86	0.58
2:J:50:THR:CG2	2:J:98:VAL:HG21	2.34	0.58
1:A:20:LEU:HD11	1:A:83:MET:HE1	1.86	0.57
1:A:74:ASN:H	1:A:74:ASN:HD22	1.51	0.57
2:J:98:VAL:CG1	2:J:99:PRO:CD	2.77	0.57
1:A:41:PRO:HB3	1:G:78:THR:OG1	2.05	0.57
1:G:20:LEU:HG	1:G:83:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD23	1:A:24:ALA:HB2	1.87	0.56
1:G:34:ILE:O	1:G:50:CYS:HB2	2.05	0.56
1:B:116:VAL:HG13	1:B:116:VAL:O	2.05	0.56
2:J:9:GLY:HA3	2:J:109:THR:HG22	1.87	0.56
1:G:4:LEU:HD23	1:G:24:ALA:HB2	1.87	0.55
1:G:64:VAL:CG1	1:G:68:PHE:HB2	2.37	0.55
1:H:9:GLY:HA2	1:H:18:LEU:HD23	1.89	0.54
3:K:11:GLU:OE1	3:L:29:ARG:NH1	2.40	0.54
1:B:12:VAL:HG21	1:B:86:LEU:HD12	1.90	0.54
1:A:35:GLY:HA2	1:A:50:CYS:HB2	1.89	0.54
3:K:36:LEU:HD11	3:L:4:GLU:HG2	1.88	0.54
2:D:9:GLY:H	2:D:109:THR:CG2	2.20	0.53
1:A:20:LEU:HG	1:A:83:MET:CE	2.36	0.53
2:J:9:GLY:N	2:J:109:THR:HG21	2.20	0.53
1:G:2:VAL:HB	1:H:106:THR:HB	1.89	0.53
2:I:33:ASP:HB3	2:I:98:VAL:CG1	2.39	0.53
2:J:28:ILE:O	2:J:34:MET:HE1	2.09	0.53
3:E:15:ILE:HG23	3:F:22:LEU:HD22	1.91	0.53
1:H:34:ILE:O	1:H:50:CYS:HB2	2.09	0.53
2:I:33:ASP:CB	2:I:98:VAL:CG1	2.87	0.53
3:L:37:LYS:O	3:L:40:LEU:HG	2.09	0.52
2:I:50:THR:OG1	2:I:98:VAL:HG21	2.10	0.52
2:J:39:GLN:C	2:J:91:ALA:HB1	2.30	0.52
2:J:44:GLN:NE2	3:K:3:GLU:HG2	2.23	0.52
1:A:12:VAL:HG11	1:A:18:LEU:HG	1.91	0.52
2:C:6:GLU:HB2	2:C:109:THR:OG1	2.10	0.52
2:J:14:PRO:HD3	2:J:114:SER:O	2.10	0.52
3:K:11:GLU:CD	3:L:29:ARG:HH11	2.13	0.52
1:G:22:CYS:HB2	1:G:36:TRP:CZ2	2.45	0.51
2:I:98:VAL:N	2:I:99:PRO:CD	2.73	0.51
2:J:39:GLN:O	2:J:91:ALA:HB1	2.11	0.51
2:D:39:GLN:C	2:D:91:ALA:HB1	2.30	0.51
1:H:64:VAL:CG1	1:H:68:PHE:HB2	2.41	0.51
1:B:13:GLN:OE1	1:B:118:SER:HB3	2.10	0.51
2:C:3:GLN:HG2	2:C:25:SER:HB2	1.90	0.51
2:C:82:MET:HE2	2:C:85:LEU:HD21	1.93	0.51
2:J:98:VAL:HG11	3:L:29:ARG:HH22	1.75	0.51
2:J:50:THR:HG21	2:J:98:VAL:HG21	1.93	0.50
1:A:11:LEU:HD12	1:A:115:THR:O	2.10	0.50
3:E:11:GLU:CD	3:F:29:ARG:NH1	2.64	0.50
2:I:82:MET:HB3	2:I:85:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:VAL:HB	1:H:18:LEU:HD11	1.93	0.50
1:H:17:SER:O	1:H:18:LEU:HD12	2.11	0.50
3:L:40:LEU:HD12	3:L:40:LEU:C	2.33	0.49
2:C:3:GLN:HG2	2:C:3:GLN:O	2.13	0.49
2:I:98:VAL:C	2:I:100:GLY:H	2.15	0.49
1:G:3:GLN:HG2	1:G:107:TYR:CD2	2.48	0.49
2:C:33:ASP:OD2	3:E:25:LYS:HE2	2.13	0.49
1:G:27:PHE:O	1:G:77:ASN:ND2	2.36	0.49
2:C:9:GLY:H	2:C:109:THR:HG21	1.78	0.49
2:D:6:GLU:HB3	2:D:109:THR:OG1	2.13	0.48
1:A:9:GLY:CA	1:A:18:LEU:HD22	2.44	0.48
2:D:9:GLY:HA3	2:D:109:THR:HG22	1.95	0.48
2:C:14:PRO:HD3	2:C:114:SER:O	2.13	0.48
1:H:12:VAL:HG13	1:H:116:VAL:HG22	1.96	0.48
2:J:44:GLN:HE21	3:K:3:GLU:HG2	1.79	0.48
3:F:4:GLU:O	3:F:8:LEU:HD23	2.14	0.48
1:A:74:ASN:ND2	1:A:74:ASN:N	2.61	0.48
1:B:68:PHE:CE2	1:B:83:MET:HG2	2.48	0.47
3:E:11:GLU:OE1	3:F:29:ARG:NH1	2.48	0.47
1:B:73:ASP:OD1	1:B:75:ALA:HB3	2.14	0.47
1:H:64:VAL:HG13	1:H:68:PHE:CG	2.49	0.47
1:A:34:ILE:HG13	1:A:79:VAL:HG21	1.96	0.47
2:C:3:GLN:HE21	2:C:3:GLN:N	2.13	0.47
2:C:98:VAL:CG1	2:C:99:PRO:HD3	2.42	0.47
2:I:101:ARG:CB	2:I:104:SER:OG	2.63	0.47
1:G:104:TYR:OH	3:L:19:LEU:HB3	2.14	0.47
1:H:20:LEU:HG	1:H:83:MET:CE	2.44	0.47
1:B:104:TYR:OH	3:E:19:LEU:HB3	2.15	0.46
2:D:88:GLU:H	2:D:88:GLU:CD	2.19	0.46
1:B:8:GLY:O	1:B:18:LEU:HD22	2.17	0.45
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.99	0.45
1:B:68:PHE:CD1	1:B:68:PHE:N	2.83	0.45
2:D:71:ARG:CD	2:D:73:ASN:OD1	2.65	0.45
1:H:64:VAL:HG13	1:H:68:PHE:HB2	1.98	0.45
2:D:12:VAL:HG11	2:D:85:LEU:HD13	1.99	0.45
2:J:12:VAL:O	2:J:113:VAL:HA	2.16	0.45
2:I:29:PHE:HE2	2:I:78:VAL:HG22	1.81	0.45
2:I:98:VAL:HG22	2:I:98:VAL:O	2.17	0.45
1:A:9:GLY:HA2	1:A:18:LEU:CD2	2.45	0.45
2:I:17:SER:HA	2:I:82:MET:O	2.17	0.45
2:D:36:TRP:CD1	2:D:80:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LEU:HD13	1:G:115:THR:OG1	2.17	0.45
1:G:119:GLY:O	1:G:120:ARG:CB	2.65	0.45
1:B:88:PRO:HA	1:B:116:VAL:CG1	2.42	0.44
1:G:91:THR:HG23	1:G:115:THR:HA	1.99	0.44
2:J:17:SER:HA	2:J:82:MET:O	2.18	0.44
2:J:29:PHE:HA	2:J:34:MET:CE	2.45	0.44
2:D:86:LYS:HB3	2:D:88:GLU:OE1	2.17	0.44
3:E:22:LEU:HB3	3:F:19:LEU:HD21	1.98	0.44
1:G:105:VAL:HG11	1:G:108:TRP:CE2	2.52	0.44
3:K:19:LEU:HD21	3:L:22:LEU:CB	2.48	0.44
1:A:64:VAL:HG13	1:A:64:VAL:O	2.17	0.44
2:D:71:ARG:HD2	2:D:73:ASN:OD1	2.17	0.44
2:I:22:CYS:O	2:I:77:THR:HG23	2.18	0.44
1:B:13:GLN:OE1	1:B:118:SER:HA	2.17	0.44
1:B:39:GLN:C	1:B:92:ALA:HB1	2.38	0.44
2:D:58:TRP:CH2	3:F:25:LYS:HG2	2.53	0.44
2:I:57:THR:O	3:L:18:GLN:NE2	2.40	0.43
2:D:47:TRP:CZ2	3:E:11:GLU:HG3	2.53	0.43
2:D:17:SER:O	2:D:18:LEU:HD23	2.18	0.43
2:D:29:PHE:CE1	2:D:76:ASN:HA	2.54	0.43
2:J:71:ARG:HD2	2:J:73:ASN:OD1	2.19	0.43
2:J:51:ILE:HG13	2:J:69:ILE:CD1	2.48	0.43
1:B:68:PHE:CE1	1:B:83:MET:HG2	2.53	0.43
3:K:5:LEU:C	3:K:5:LEU:HD23	2.38	0.43
3:E:8:LEU:HD23	3:E:8:LEU:HA	1.78	0.43
2:J:22:CYS:HB3	2:J:78:VAL:HG13	2.01	0.42
2:J:33:ASP:OD2	3:L:25:LYS:HE2	2.19	0.42
1:H:20:LEU:HD11	1:H:83:MET:HE1	2.01	0.42
1:B:22:CYS:HB2	1:B:36:TRP:CZ2	2.54	0.42
2:C:44:GLN:OE1	3:F:3:GLU:HA	2.19	0.42
2:J:9:GLY:H	2:J:109:THR:CG2	2.23	0.42
2:J:47:TRP:HE1	2:J:50:THR:HG1	1.67	0.42
2:C:32:ASN:O	2:C:71:ARG:NH2	2.43	0.42
2:C:98:VAL:HG11	3:E:29:ARG:CZ	2.46	0.42
2:C:6:GLU:HG3	2:C:108:GLY:HA2	2.02	0.42
2:D:113:VAL:O	2:D:114:SER:HB3	2.19	0.42
2:I:33:ASP:OD2	3:K:25:LYS:NZ	2.50	0.42
2:J:50:THR:HG23	2:J:98:VAL:HG21	2.02	0.42
2:J:51:ILE:HG13	2:J:69:ILE:HD13	2.01	0.42
2:J:72:ASP:OD2	2:J:75:LYS:HE2	2.20	0.42
3:L:36:LEU:HD12	3:L:36:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:ASP:HB2	2:J:98:VAL:HG12	1.99	0.41
2:J:101:ARG:C	2:J:103:GLY:H	2.23	0.41
2:J:82:MET:HE2	2:J:85:LEU:HD21	2.00	0.41
2:C:24:ALA:CB	2:C:29:PHE:HB2	2.50	0.41
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.53	0.41
1:B:68:PHE:N	1:B:68:PHE:HD1	2.18	0.41
2:C:71:ARG:HD3	2:C:73:ASN:OD1	2.20	0.41
2:D:82:MET:HE2	2:D:85:LEU:HD21	2.01	0.41
2:D:17:SER:HA	2:D:82:MET:O	2.20	0.41
1:G:64:VAL:CG1	1:G:68:PHE:CG	3.01	0.41
3:K:36:LEU:HB3	3:L:5:LEU:HD12	2.02	0.41
1:G:3:GLN:HG2	1:G:107:TYR:CE2	2.56	0.41
2:C:6:GLU:HA	2:C:21:SER:O	2.21	0.41
2:J:28:ILE:O	2:J:34:MET:CE	2.69	0.41
1:A:40:ALA:HB1	1:A:41:PRO:CD	2.51	0.41
1:B:83:MET:HB3	1:B:86:LEU:HD21	2.03	0.41
3:F:8:LEU:HD13	3:F:8:LEU:HA	1.94	0.40
2:J:50:THR:HG23	2:J:98:VAL:CG2	2.51	0.40
2:I:83:ASN:O	2:I:84:ASP:C	2.60	0.40
2:C:71:ARG:CD	2:C:73:ASN:OD1	2.70	0.40
3:E:22:LEU:HD23	3:E:22:LEU:HA	1.86	0.40
2:I:38:ARG:HD3	2:I:48:VAL:HG21	2.03	0.40
3:F:19:LEU:HD23	3:F:19:LEU:HA	1.95	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	116/133 (87%)	112 (97%)	4 (3%)	0	100	100
1	B	115/133 (86%)	109 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	118/133 (89%)	115 (98%)	3 (2%)	0	100 100
1	H	114/133 (86%)	110 (96%)	4 (4%)	0	100 100
2	C	111/130 (85%)	107 (96%)	4 (4%)	0	100 100
2	D	110/130 (85%)	106 (96%)	4 (4%)	0	100 100
2	I	112/130 (86%)	105 (94%)	6 (5%)	1 (1%)	17 40
2	J	111/130 (85%)	103 (93%)	8 (7%)	0	100 100
3	E	40/42 (95%)	40 (100%)	0	0	100 100
3	F	39/42 (93%)	39 (100%)	0	0	100 100
3	K	38/42 (90%)	38 (100%)	0	0	100 100
3	L	38/42 (90%)	38 (100%)	0	0	100 100
All	All	1062/1220 (87%)	1022 (96%)	39 (4%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	98	VAL

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	94/107 (88%)	92 (98%)	2 (2%)	53 80
1	B	94/107 (88%)	92 (98%)	2 (2%)	53 80
1	G	94/107 (88%)	94 (100%)	0	100 100
1	H	94/107 (88%)	94 (100%)	0	100 100
2	C	89/105 (85%)	86 (97%)	3 (3%)	37 66
2	D	89/105 (85%)	86 (97%)	3 (3%)	37 66
2	I	89/105 (85%)	89 (100%)	0	100 100
2	J	86/105 (82%)	84 (98%)	2 (2%)	50 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	34/35 (97%)	34 (100%)	0	100 100
3	F	31/35 (89%)	30 (97%)	1 (3%)	39 68
3	K	32/35 (91%)	30 (94%)	2 (6%)	18 40
3	L	35/35 (100%)	34 (97%)	1 (3%)	42 71
All	All	861/988 (87%)	845 (98%)	16 (2%)	57 82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	89	GLU
1	B	89	GLU
1	B	91	THR
2	C	3	GLN
2	C	6	GLU
2	C	95	CYS
2	D	95	CYS
2	D	98	VAL
2	D	109	THR
3	F	29	ARG
2	J	3	GLN
2	J	95	CYS
3	K	10	GLU
3	K	13	GLN
3	L	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	74	ASN
2	J	44	GLN

5.3.3 RNA

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)

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	EDO	A	201	-	3,3,3	0.34	0	2,2,2	0.30	0
4	EDO	H	201	-	3,3,3	0.25	0	2,2,2	0.42	0
6	ACT	G	201	-	1,3,3	2.46	1 (100%)	0,3,3	0.00	-
5	GOL	D	201	-	5,5,5	1.33	1 (20%)	5,5,5	0.45	0
4	EDO	B	201	-	3,3,3	0.26	0	2,2,2	0.57	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
4	EDO	A	201	-	-	1/1/1/1	-
5	GOL	D	201	-	-	4/4/4/4	-
4	EDO	H	201	-	-	0/1/1/1	-
4	EDO	B	201	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	ACT	CH3-C	2.46	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	201	GOL	C3-C2	2.01	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	201	GOL	C1-C2-C3-O3
5	D	201	GOL	O2-C2-C3-O3
5	D	201	GOL	O1-C1-C2-C3
5	D	201	GOL	O1-C1-C2-O2
4	A	201	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	118/133 (88%)	-0.22	1 (0%) 86 87	45, 63, 108, 122	0
1	B	117/133 (87%)	0.21	4 (3%) 45 45	48, 79, 118, 140	0
1	G	120/133 (90%)	-0.21	0 100 100	44, 66, 111, 139	0
1	H	116/133 (87%)	-0.24	0 100 100	43, 62, 87, 125	0
2	C	113/130 (86%)	0.24	5 (4%) 34 33	55, 87, 117, 146	0
2	D	112/130 (86%)	0.00	2 (1%) 68 70	30, 70, 106, 117	0
2	I	113/130 (86%)	0.00	5 (4%) 34 33	51, 70, 104, 117	0
2	J	113/130 (86%)	0.20	7 (6%) 20 19	53, 96, 132, 155	0
3	E	40/42 (95%)	-0.10	0 100 100	50, 63, 123, 146	0
3	F	40/42 (95%)	-0.35	0 100 100	47, 68, 105, 132	0
3	K	40/42 (95%)	-0.10	1 (2%) 57 59	45, 66, 134, 151	0
3	L	40/42 (95%)	-0.17	0 100 100	45, 64, 116, 119	0
All	All	1082/1220 (88%)	-0.03	25 (2%) 60 62	30, 72, 117, 155	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	114	SER	4.4
2	C	114	SER	4.3
2	I	98	VAL	4.1
2	J	14	PRO	3.8
2	J	115	SER	3.7
2	C	98	VAL	3.5
2	D	13	GLN	3.1
2	J	13	GLN	3.1
2	J	98	VAL	3.0
2	I	4	LEU	3.0
2	J	11	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	27	PHE	2.6
1	B	10	GLY	2.5
3	K	1	LEU	2.5
1	B	43	LYS	2.4
2	J	113	VAL	2.4
2	D	98	VAL	2.4
2	C	11	LEU	2.4
2	I	26	GLY	2.4
1	A	27	PHE	2.4
2	I	53[A]	TYR	2.2
2	I	27	SER	2.1
2	C	101	ARG	2.1
2	C	115	SER	2.1
1	B	18	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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(Å^2)	Q<0.9
4	EDO	H	201	4/4	0.76	0.20	87,105,113,113	0
5	GOL	D	201	6/6	0.85	0.20	88,107,129,129	0
4	EDO	B	201	4/4	0.87	0.24	94,113,120,120	0
6	ACT	G	201	4/4	0.89	0.17	88,91,106,106	0
4	EDO	A	201	4/4	0.93	0.25	80,97,105,106	0

6.5 Other polymers (i)

There are no such residues in this entry.