Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:44 am BST

PDB ID	:	5WY5
Title	:	Crystal structure of MAGEG1 and NSE1 complex
Authors	:	Yang, M.; Gao, J.
Deposited on	:	2017-01-11
Resolution	:	2.92 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:

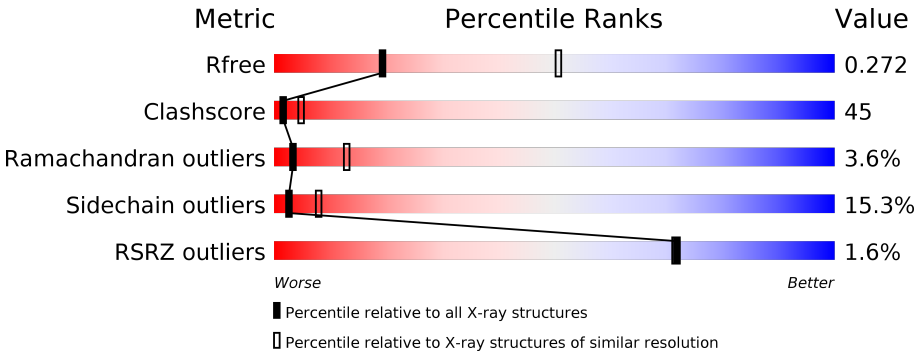
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 <=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	B	217	3%, 28%, 46%, 12%, ·, 13%
2	A	238	37%, 53%, 8%, ··

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3483 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 Melanoma-associated antigen G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	189	Total	C	N	O	S	0	0	0
			1549	1003	265	276	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	193	LEU	ILE	engineered mutation	UNP Q96MG7
B	258	LEU	THR	engineered mutation	UNP Q96MG7

- Molecule 2 is a protein called Non-structural maintenance of chromosomes element 1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	236	Total	C	N	O	S	0	0	0
			1913	1212	329	358	14			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	O	0	0
			5	5		

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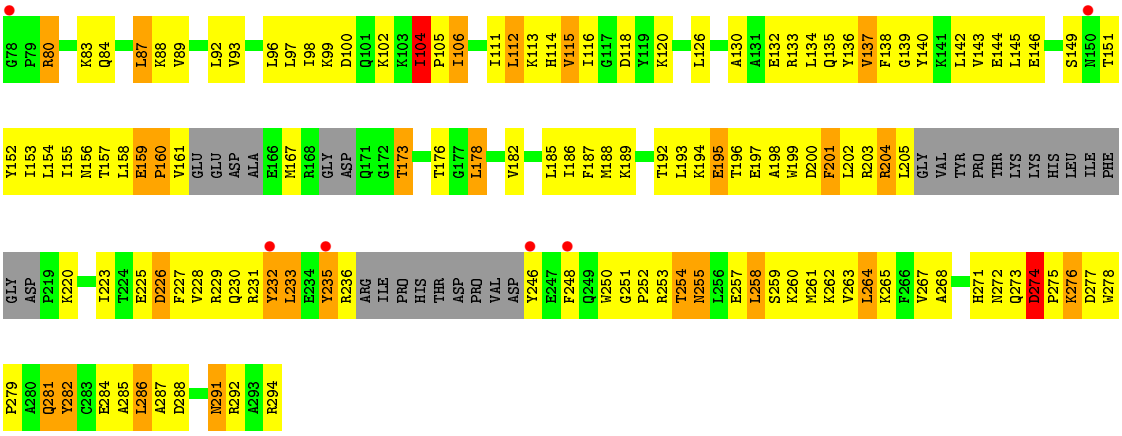
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		

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.

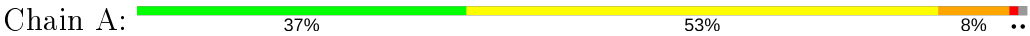
- Molecule 1: Melanoma-associated antigen G1

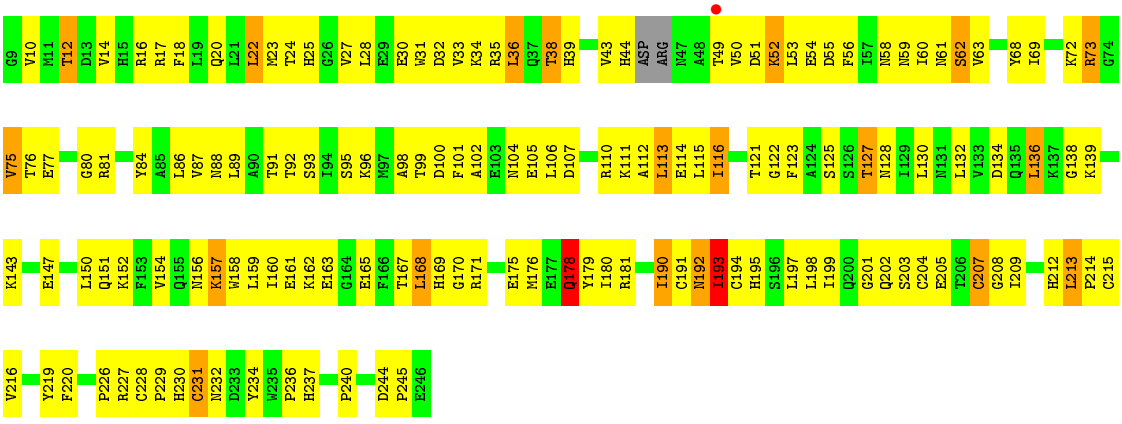
Chain B:



- Molecule 2: Non-structural maintenance of chromosomes element 1 homolog

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.26Å 154.33Å 53.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.36 – 2.92 32.36 – 2.92	Depositor EDS
% Data completeness (in resolution range)	91.1 (32.36-2.92) 97.4 (32.36-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.216 , 0.270 0.231 , 0.272	Depositor DCC
R_{free} test set	756 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.3	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	0.94	EDS
Total number of atoms	3483	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.41	0/1577	0.64	0/2120
2	A	0.40	0/1950	0.59	0/2633
All	All	0.41	0/3527	0.61	0/4753

There are no bond length outliers.

There are no bond angle outliers.

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	B	1549	0	1578	178	0
2	A	1913	0	1895	144	0
3	B	2	0	0	0	0
4	A	2	0	0	0	0
5	A	12	0	0	3	0
5	B	5	0	0	0	0
All	All	3483	0	3473	312	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 45.

All (312) 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:B:158:LEU:HB3	1:B:159:GLU:HB2	1.37	1.02
1:B:186:ILE:HA	1:B:193:LEU:HD13	1.39	1.02
1:B:255:ASN:H	1:B:255:ASN:ND2	1.61	0.96
2:A:191:CYS:HB2	2:A:212:HIS:CD2	2.01	0.95
1:B:159:GLU:H	1:B:160:PRO:CA	1.81	0.93
1:B:274:ASP:H	1:B:275:PRO:HD3	1.30	0.93
1:B:250:TRP:CH2	1:B:263:VAL:HG21	2.07	0.90
1:B:255:ASN:HD22	1:B:255:ASN:H	1.16	0.89
2:A:121:THR:HG22	2:A:123:PHE:HD1	1.37	0.88
2:A:198:LEU:HA	2:A:212:HIS:CE1	2.08	0.87
2:A:198:LEU:HA	2:A:212:HIS:HE1	1.40	0.86
1:B:268:ALA:HB1	1:B:273:GLN:O	1.76	0.84
1:B:230:GLN:HB2	1:B:253:ARG:HD2	1.62	0.80
1:B:143:VAL:HG12	1:B:144:GLU:O	1.82	0.79
1:B:198:ALA:O	1:B:201:PHE:HD1	1.66	0.79
2:A:95:SER:HA	2:A:98:ALA:HB3	1.66	0.77
1:B:282:TYR:HE1	1:B:286:LEU:HD23	1.50	0.76
1:B:158:LEU:CB	1:B:159:GLU:HB2	2.14	0.76
1:B:274:ASP:H	1:B:275:PRO:CD	1.99	0.75
2:A:101:PHE:HB2	2:A:106:LEU:HD23	1.68	0.75
1:B:160:PRO:O	1:B:161:VAL:HB	1.88	0.73
1:B:100:ASP:CG	1:B:154:LEU:HB2	2.08	0.73
2:A:20:GLN:O	2:A:24:THR:HG23	1.87	0.73
1:B:159:GLU:N	1:B:160:PRO:HA	2.04	0.73
2:A:113:LEU:HD23	2:A:113:LEU:C	2.08	0.73
1:B:201:PHE:C	1:B:201:PHE:CD1	2.62	0.73
1:B:259:SER:O	1:B:263:VAL:HG23	1.89	0.72
2:A:12:THR:HB	2:A:14:VAL:HG22	1.71	0.72
2:A:52:LYS:HD2	2:A:54:GLU:H	1.55	0.72
1:B:159:GLU:N	1:B:160:PRO:CA	2.51	0.72
2:A:198:LEU:HB2	2:A:212:HIS:NE2	2.05	0.71
1:B:142:LEU:HD11	1:B:152:TYR:HB3	1.71	0.71
2:A:101:PHE:HB2	2:A:106:LEU:CD2	2.20	0.71
1:B:133:ARG:HA	1:B:133:ARG:HH11	1.55	0.70
1:B:198:ALA:O	1:B:201:PHE:CD1	2.44	0.70
1:B:278:TRP:O	1:B:282:TYR:N	2.24	0.70
1:B:272:ASN:O	1:B:273:GLN:HG2	1.92	0.69
1:B:104:ILE:HB	1:B:105:PRO:C	2.14	0.69
1:B:192:THR:C	1:B:193:LEU:HD12	2.13	0.69
1:B:250:TRP:HH2	1:B:263:VAL:HG21	1.55	0.69
1:B:159:GLU:H	1:B:160:PRO:CB	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:HD23	1:B:116:ILE:HB	1.75	0.68
2:A:121:THR:HG22	2:A:123:PHE:CD1	2.26	0.68
2:A:52:LYS:NZ	5:A:401:HOH:O	2.25	0.68
1:B:281:GLN:O	1:B:284:GLU:HG2	1.94	0.67
1:B:204:ARG:HD2	1:B:205:LEU:CD1	2.25	0.67
2:A:75:VAL:HG23	2:A:80:GLY:HA2	1.76	0.66
2:A:198:LEU:HB2	2:A:212:HIS:CE1	2.31	0.66
1:B:159:GLU:H	1:B:160:PRO:HA	1.58	0.65
1:B:231:ARG:HH12	1:B:257:GLU:CD	2.00	0.65
2:A:31:TRP:CZ3	2:A:35:ARG:HD2	2.32	0.64
2:A:228:CYS:SG	2:A:230:HIS:O	2.56	0.64
2:A:50:VAL:HG23	2:A:50:VAL:O	1.96	0.64
1:B:102:LYS:HB3	1:B:104:ILE:HD13	1.80	0.64
1:B:202:LEU:HD13	1:B:202:LEU:C	2.18	0.64
2:A:176:MET:HE2	5:A:405:HOH:O	1.97	0.64
1:B:231:ARG:O	1:B:250:TRP:O	2.15	0.64
1:B:255:ASN:HD22	1:B:255:ASN:N	1.94	0.64
2:A:219:TYR:CE2	2:A:229:PRO:HG3	2.33	0.63
2:A:28:LEU:HB2	2:A:33:VAL:HG12	1.80	0.63
2:A:198:LEU:CA	2:A:212:HIS:CE1	2.79	0.63
2:A:102:ALA:O	2:A:106:LEU:HG	1.99	0.62
1:B:272:ASN:O	1:B:273:GLN:CG	2.47	0.62
1:B:275:PRO:O	1:B:279:PRO:HG3	1.99	0.62
2:A:77:GLU:OE1	2:A:199:ILE:HB	1.98	0.62
2:A:201:GLY:HA2	2:A:213:LEU:HD13	1.81	0.62
1:B:104:ILE:HB	1:B:105:PRO:CA	2.30	0.62
1:B:225:GLU:O	1:B:228:VAL:HB	2.00	0.62
1:B:145:LEU:HD23	1:B:145:LEU:H	1.64	0.61
2:A:198:LEU:CB	2:A:212:HIS:CE1	2.84	0.61
1:B:92:LEU:CD2	1:B:96:LEU:HD11	2.30	0.60
1:B:273:GLN:O	1:B:274:ASP:HB3	2.02	0.60
2:A:213:LEU:HB2	2:A:214:PRO:HD3	1.83	0.60
2:A:228:CYS:O	2:A:232:ASN:HA	2.00	0.60
1:B:255:ASN:N	1:B:255:ASN:ND2	2.40	0.59
2:A:169:HIS:ND1	2:A:170:GLY:N	2.50	0.59
1:B:233:LEU:HD22	1:B:251:GLY:HA2	1.84	0.59
2:A:95:SER:HA	2:A:98:ALA:CB	2.32	0.59
1:B:287:ALA:O	1:B:291:ASN:HB2	2.03	0.59
2:A:158:TRP:HZ3	2:A:175:GLU:HG3	1.68	0.59
1:B:159:GLU:HA	1:B:159:GLU:OE1	2.03	0.59
2:A:143:LYS:O	2:A:147:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TRP:N	1:B:279:PRO:HD3	2.18	0.58
1:B:259:SER:OG	1:B:262:LYS:HG3	2.03	0.58
2:A:100:ASP:HB3	2:A:101:PHE:CD1	2.39	0.58
1:B:99:LYS:HB3	1:B:104:ILE:HG13	1.86	0.58
1:B:132:GLU:HG3	1:B:133:ARG:H	1.69	0.58
2:A:191:CYS:HB2	2:A:212:HIS:HD2	1.60	0.58
1:B:149:SER:HB3	1:B:151:THR:OG1	2.04	0.57
1:B:276:LYS:HE3	1:B:277:ASP:HB3	1.86	0.57
2:A:194:CYS:O	2:A:195:HIS:HB2	2.05	0.57
2:A:107:ASP:O	2:A:111:LYS:HG2	2.04	0.56
2:A:39:HIS:CE1	2:A:43:VAL:HG21	2.40	0.56
2:A:87:VAL:HG22	2:A:175:GLU:HA	1.86	0.56
1:B:143:VAL:HG21	1:B:155:ILE:HD12	1.86	0.56
1:B:258:LEU:HG	1:B:262:LYS:HD2	1.87	0.56
1:B:265:LYS:O	1:B:268:ALA:HB3	2.05	0.56
1:B:158:LEU:HD12	2:A:20:GLN:OE1	2.06	0.56
1:B:236:ARG:HD2	1:B:246:TYR:CE1	2.41	0.56
2:A:220:PHE:CD1	2:A:226:PRO:HB3	2.41	0.56
1:B:142:LEU:CD1	1:B:152:TYR:HB3	2.35	0.56
1:B:161:VAL:C	2:A:17:ARG:HH22	2.08	0.56
2:A:112:ALA:O	2:A:116:ILE:HG12	2.05	0.56
2:A:121:THR:CG2	2:A:123:PHE:HD1	2.16	0.55
1:B:133:ARG:O	1:B:137:VAL:HG13	2.07	0.55
1:B:276:LYS:HG3	1:B:277:ASP:N	2.22	0.54
2:A:10:VAL:HG23	2:A:10:VAL:O	2.07	0.54
1:B:254:THR:O	1:B:257:GLU:N	2.36	0.54
1:B:144:GLU:HG2	1:B:149:SER:HB2	1.88	0.54
1:B:160:PRO:O	1:B:161:VAL:CB	2.55	0.54
2:A:192:ASN:C	2:A:193:ILE:HG12	2.27	0.54
2:A:98:ALA:HA	2:A:106:LEU:HD13	1.90	0.54
1:B:113:LYS:HD3	1:B:114:HIS:NE2	2.22	0.54
2:A:73:ARG:HG3	2:A:84:TYR:CZ	2.43	0.53
1:B:133:ARG:NH1	1:B:136:TYR:HB3	2.23	0.53
1:B:178:LEU:O	1:B:182:VAL:HG23	2.07	0.53
2:A:160:ILE:HB	2:A:167:THR:HG22	1.90	0.53
2:A:191:CYS:SG	2:A:192:ASN:O	2.66	0.53
1:B:138:PHE:CE2	2:A:23:MET:HE1	2.43	0.53
2:A:18:PHE:CD1	2:A:36:LEU:HD13	2.43	0.53
1:B:230:GLN:HB2	1:B:253:ARG:CD	2.34	0.53
2:A:28:LEU:CB	2:A:33:VAL:HG12	2.38	0.52
1:B:204:ARG:HG2	1:B:205:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:MET:HE1	1:B:286:LEU:HA	1.91	0.52
2:A:27:VAL:O	2:A:28:LEU:HD23	2.09	0.52
2:A:18:PHE:CE1	2:A:36:LEU:HD13	2.45	0.52
1:B:135:GLN:O	1:B:139:GLY:HA2	2.09	0.52
1:B:137:VAL:HG13	1:B:138:PHE:CE1	2.44	0.52
1:B:201:PHE:HA	1:B:204:ARG:NH1	2.24	0.52
2:A:98:ALA:HA	2:A:106:LEU:CD1	2.39	0.52
1:B:173:THR:OG1	1:B:176:THR:HG22	2.08	0.52
2:A:77:GLU:OE2	2:A:212:HIS:CE1	2.63	0.52
1:B:89:VAL:O	1:B:93:VAL:HG13	2.09	0.52
2:A:227:ARG:NH2	2:A:234:TYR:CE1	2.78	0.52
1:B:133:ARG:O	1:B:137:VAL:CG1	2.58	0.52
1:B:233:LEU:HD13	1:B:252:PRO:HD3	1.92	0.52
1:B:273:GLN:OE1	1:B:275:PRO:HD2	2.10	0.52
1:B:142:LEU:HD11	1:B:152:TYR:CB	2.39	0.51
1:B:273:GLN:HE22	1:B:276:LYS:HG2	1.75	0.51
1:B:202:LEU:O	1:B:203:ARG:C	2.47	0.51
1:B:276:LYS:C	1:B:279:PRO:HD3	2.31	0.51
2:A:113:LEU:CD2	2:A:113:LEU:C	2.79	0.51
2:A:52:LYS:NZ	2:A:54:GLU:HB2	2.26	0.51
1:B:282:TYR:CE1	1:B:286:LEU:HD23	2.38	0.51
2:A:34:LYS:NZ	2:A:53:LEU:H	2.09	0.51
1:B:111:ILE:O	1:B:115:VAL:HG22	2.11	0.51
2:A:244:ASP:OD1	2:A:245:PRO:HD2	2.11	0.51
2:A:73:ARG:HG3	2:A:84:TYR:CE2	2.46	0.50
1:B:204:ARG:HD2	1:B:205:LEU:HD12	1.92	0.50
2:A:216:VAL:CG2	2:A:240:PRO:HD2	2.41	0.50
2:A:156:ASN:O	2:A:157:LYS:HB2	2.10	0.50
1:B:278:TRP:N	1:B:279:PRO:CD	2.75	0.50
2:A:157:LYS:O	2:A:171:ARG:HB3	2.12	0.50
1:B:115:VAL:CG2	1:B:116:ILE:N	2.74	0.50
1:B:195:GLU:OE1	1:B:246:TYR:CD2	2.64	0.50
2:A:52:LYS:HZ1	2:A:54:GLU:HB2	1.77	0.49
1:B:93:VAL:O	1:B:97:LEU:HG	2.10	0.49
1:B:99:LYS:HA	1:B:104:ILE:HD11	1.93	0.49
2:A:158:TRP:CZ3	2:A:175:GLU:HG3	2.46	0.49
1:B:173:THR:O	1:B:176:THR:HG22	2.13	0.49
1:B:161:VAL:C	2:A:17:ARG:NH2	2.66	0.49
1:B:113:LYS:CE	1:B:114:HIS:CE1	2.96	0.49
2:A:50:VAL:O	2:A:50:VAL:CG2	2.60	0.49
1:B:116:ILE:HG21	1:B:120:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:TYR:CZ	2:A:20:GLN:NE2	2.80	0.49
1:B:188:MET:HA	1:B:281:GLN:NE2	2.28	0.49
2:A:111:LYS:HB3	2:A:132:LEU:HD13	1.95	0.49
1:B:83:LYS:HG2	1:B:87:LEU:HD22	1.94	0.49
1:B:132:GLU:HG3	1:B:133:ARG:N	2.27	0.49
1:B:231:ARG:HA	1:B:253:ARG:HB3	1.94	0.49
2:A:207:CYS:HB3	2:A:209:ILE:H	1.78	0.48
2:A:212:HIS:O	2:A:215:CYS:N	2.46	0.48
1:B:278:TRP:O	1:B:281:GLN:N	2.46	0.48
2:A:122:GLY:HA3	2:A:199:ILE:O	2.13	0.48
2:A:110:ARG:O	2:A:114:GLU:HG3	2.13	0.48
2:A:191:CYS:O	2:A:195:HIS:HA	2.13	0.48
2:A:192:ASN:O	2:A:194:CYS:N	2.46	0.48
1:B:98:ILE:HG21	2:A:99:THR:HB	1.96	0.48
1:B:284:GLU:O	1:B:288:ASP:N	2.46	0.48
2:A:69:ILE:HG22	2:A:88:ASN:HA	1.96	0.48
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.69	0.48
1:B:186:ILE:HD12	1:B:232:TYR:CE1	2.49	0.47
1:B:80:ARG:HA	1:B:84:GLN:OE1	2.14	0.47
2:A:56:PHE:O	2:A:59:ASN:HB3	2.14	0.47
1:B:192:THR:O	1:B:193:LEU:HD12	2.13	0.47
1:B:235:TYR:O	1:B:246:TYR:HA	2.13	0.47
1:B:271:HIS:O	1:B:272:ASN:CG	2.53	0.47
1:B:201:PHE:CD1	1:B:202:LEU:N	2.82	0.47
1:B:258:LEU:HG	1:B:259:SER:H	1.79	0.47
1:B:92:LEU:HD22	1:B:96:LEU:HD11	1.96	0.47
2:A:30:GLU:HG3	2:A:84:TYR:CE1	2.49	0.47
2:A:93:SER:O	2:A:176:MET:HG2	2.13	0.47
1:B:99:LYS:CA	1:B:104:ILE:HD11	2.44	0.47
2:A:230:HIS:O	2:A:231:CYS:CB	2.62	0.47
1:B:258:LEU:HD23	1:B:263:VAL:CG2	2.44	0.47
2:A:125:SER:OG	2:A:128:ASN:HB2	2.14	0.47
1:B:113:LYS:HD3	1:B:114:HIS:CE1	2.50	0.47
2:A:178:GLN:CG	2:A:179:TYR:H	2.28	0.47
1:B:146:GLU:HB2	1:B:149:SER:OG	2.15	0.47
2:A:176:MET:O	2:A:180:ILE:HG13	2.15	0.47
1:B:188:MET:HA	1:B:281:GLN:HE22	1.79	0.47
1:B:102:LYS:HB3	1:B:104:ILE:CD1	2.44	0.47
2:A:36:LEU:O	2:A:39:HIS:HB3	2.14	0.46
1:B:199:TRP:CZ2	1:B:203:ARG:NH1	2.83	0.46
2:A:39:HIS:ND1	2:A:39:HIS:C	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PHE:HB2	1:B:250:TRP:CZ2	2.50	0.46
2:A:100:ASP:HB3	2:A:101:PHE:CE1	2.50	0.46
1:B:271:HIS:O	1:B:272:ASN:OD1	2.33	0.46
1:B:268:ALA:HB1	1:B:274:ASP:HB3	1.97	0.46
1:B:203:ARG:O	1:B:204:ARG:C	2.53	0.46
1:B:132:GLU:CG	1:B:133:ARG:N	2.78	0.46
2:A:30:GLU:HG3	2:A:84:TYR:HE1	1.81	0.46
1:B:294:ARG:O	1:B:294:ARG:HG2	2.16	0.45
2:A:168:LEU:HA	2:A:168:LEU:HD12	1.70	0.45
1:B:159:GLU:H	1:B:160:PRO:HB3	1.80	0.45
2:A:22:LEU:O	2:A:25:HIS:O	2.34	0.45
2:A:96:LYS:HD2	2:A:175:GLU:OE1	2.16	0.45
2:A:198:LEU:HD23	2:A:198:LEU:C	2.37	0.45
2:A:216:VAL:HG22	2:A:240:PRO:HD2	1.98	0.45
1:B:89:VAL:HG12	1:B:126:LEU:HD12	1.99	0.45
1:B:226:ASP:C	1:B:228:VAL:N	2.69	0.45
2:A:34:LYS:HZ2	2:A:53:LEU:H	1.65	0.45
1:B:268:ALA:CB	1:B:274:ASP:HB3	2.47	0.44
1:B:138:PHE:N	1:B:138:PHE:CD1	2.85	0.44
1:B:153:ILE:HG12	1:B:154:LEU:H	1.82	0.44
2:A:202:GLN:HG3	2:A:213:LEU:HD12	1.98	0.44
1:B:194:LYS:HB2	1:B:197:GLU:OE2	2.17	0.44
1:B:278:TRP:O	1:B:279:PRO:C	2.55	0.44
2:A:111:LYS:O	2:A:115:LEU:HG	2.18	0.44
2:A:127:THR:HA	2:A:130:LEU:HD12	2.00	0.44
2:A:102:ALA:HB3	2:A:105:GLU:HG3	2.00	0.44
1:B:185:LEU:HD21	1:B:201:PHE:CZ	2.53	0.44
2:A:213:LEU:CB	2:A:214:PRO:HD3	2.47	0.44
2:A:228:CYS:O	2:A:232:ASN:N	2.49	0.44
2:A:14:VAL:HG12	2:A:44:HIS:HB2	1.99	0.44
2:A:52:LYS:O	2:A:55:ASP:N	2.50	0.44
1:B:278:TRP:C	1:B:282:TYR:HB2	2.38	0.44
2:A:101:PHE:HB2	2:A:106:LEU:HD21	1.97	0.44
2:A:157:LYS:HA	2:A:169:HIS:CD2	2.53	0.44
2:A:207:CYS:CB	2:A:209:ILE:H	2.31	0.44
2:A:54:GLU:O	2:A:58:ASN:ND2	2.50	0.44
2:A:121:THR:CG2	2:A:123:PHE:CD1	2.98	0.44
2:A:191:CYS:C	2:A:192:ASN:O	2.53	0.44
2:A:16:ARG:O	2:A:20:GLN:HG3	2.18	0.43
1:B:92:LEU:HD23	1:B:92:LEU:O	2.18	0.43
2:A:38:THR:CG2	2:A:39:HIS:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:HE22	1:B:157:THR:HG21	1.84	0.43
1:B:288:ASP:O	1:B:292:ARG:HG2	2.18	0.43
2:A:72:LYS:O	2:A:84:TYR:HA	2.18	0.43
2:A:161:GLU:HG3	2:A:165:GLU:O	2.19	0.43
2:A:34:LYS:HD2	2:A:53:LEU:HB2	2.00	0.43
2:A:76:THR:HG23	2:A:81:ARG:O	2.19	0.43
1:B:161:VAL:O	1:B:161:VAL:HG22	2.18	0.43
1:B:185:LEU:HD11	1:B:201:PHE:CZ	2.54	0.43
2:A:96:LYS:HE2	5:A:407:HOH:O	2.18	0.43
1:B:133:ARG:HH12	1:B:136:TYR:HB3	1.83	0.43
1:B:100:ASP:HB2	1:B:154:LEU:HD22	2.00	0.43
1:B:268:ALA:O	1:B:272:ASN:N	2.51	0.43
1:B:115:VAL:HG23	1:B:116:ILE:N	2.34	0.43
1:B:185:LEU:HA	1:B:188:MET:HE2	2.01	0.43
1:B:250:TRP:CZ2	1:B:263:VAL:HG21	2.50	0.43
1:B:278:TRP:CB	1:B:282:TYR:HB2	2.48	0.43
2:A:212:HIS:O	2:A:215:CYS:HB2	2.19	0.43
1:B:201:PHE:HD1	1:B:202:LEU:N	2.16	0.43
1:B:264:LEU:HA	1:B:267:VAL:HG22	2.00	0.43
2:A:113:LEU:HA	2:A:116:ILE:HG13	1.99	0.42
1:B:87:LEU:HA	1:B:87:LEU:HD12	1.72	0.42
2:A:167:THR:HG23	2:A:168:LEU:O	2.19	0.42
1:B:275:PRO:O	1:B:279:PRO:HD3	2.20	0.42
2:A:60:ILE:C	2:A:62:SER:N	2.72	0.42
2:A:181:ARG:HH11	2:A:190:ILE:CG2	2.32	0.42
1:B:138:PHE:HE2	2:A:23:MET:HE1	1.85	0.42
2:A:75:VAL:CG2	2:A:80:GLY:HA2	2.47	0.42
2:A:75:VAL:HG23	2:A:80:GLY:CA	2.48	0.42
1:B:276:LYS:CG	1:B:277:ASP:N	2.82	0.42
1:B:275:PRO:O	1:B:279:PRO:CD	2.67	0.42
2:A:160:ILE:CD1	2:A:169:HIS:HA	2.50	0.42
2:A:207:CYS:HB3	2:A:208:GLY:H	1.70	0.42
2:A:197:LEU:O	2:A:212:HIS:CE1	2.73	0.42
2:A:32:ASP:O	2:A:36:LEU:HB2	2.20	0.42
1:B:186:ILE:CD1	1:B:248:PHE:HB3	2.49	0.42
2:A:159:LEU:HA	2:A:159:LEU:HD23	1.75	0.42
1:B:134:LEU:HA	1:B:134:LEU:HD12	1.82	0.42
2:A:104:ASN:HB3	2:A:138:GLY:O	2.20	0.41
1:B:106:ILE:HG12	1:B:152:TYR:O	2.20	0.41
1:B:258:LEU:HG	1:B:262:LYS:HB2	2.01	0.41
1:B:186:ILE:HG21	1:B:250:TRP:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:HD2	1:B:276:LYS:C	2.41	0.41
2:A:162:LYS:C	2:A:163:GLU:HG2	2.40	0.41
1:B:138:PHE:HD2	2:A:23:MET:HE3	1.85	0.41
1:B:153:ILE:HG12	1:B:154:LEU:N	2.36	0.41
1:B:258:LEU:HD23	1:B:263:VAL:HG23	2.02	0.41
2:A:228:CYS:O	2:A:232:ASN:CA	2.67	0.41
2:A:236:PRO:HG2	2:A:237:HIS:CD2	2.55	0.41
1:B:275:PRO:O	1:B:279:PRO:CG	2.67	0.41
1:B:130:ALA:O	1:B:134:LEU:HB2	2.21	0.41
1:B:273:GLN:HB2	1:B:275:PRO:HD3	2.03	0.41
1:B:282:TYR:O	1:B:285:ALA:N	2.54	0.41
2:A:204:CYS:HB3	2:A:207:CYS:HB2	2.03	0.41
2:A:60:ILE:O	2:A:61:ASN:C	2.59	0.41
2:A:101:PHE:HE2	2:A:152:LYS:CD	2.34	0.40
1:B:83:LYS:HD2	2:A:68:TYR:CE2	2.56	0.40
2:A:203:SER:HA	2:A:209:ILE:O	2.21	0.40
1:B:228:VAL:O	1:B:229:ARG:C	2.59	0.40
1:B:258:LEU:CD2	1:B:263:VAL:HG22	2.51	0.40
1:B:274:ASP:N	1:B:275:PRO:CD	2.75	0.40
2:A:150:LEU:O	2:A:154:VAL:HG23	2.22	0.40
1:B:138:PHE:CD2	2:A:23:MET:HE3	2.56	0.40
1:B:189:LYS:HB3	1:B:193:LEU:CG	2.51	0.40
2:A:58:ASN:H	2:A:58:ASN:HD22	1.70	0.40
1:B:260:LYS:HG3	1:B:288:ASP:OD2	2.20	0.40
1:B:99:LYS:HB3	1:B:104:ILE:CG1	2.52	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	B	179/217 (82%)	150 (84%)	21 (12%)	8 (4%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	232/238 (98%)	206 (89%)	19 (8%)	7 (3%)	4 16
All	All	411/455 (90%)	356 (87%)	40 (10%)	15 (4%)	3 13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	GLU
1	B	160	PRO
1	B	204	ARG
1	B	274	ASP
2	A	207	CYS
2	A	193	ILE
1	B	220	LYS
2	A	136	LEU
2	A	192	ASN
1	B	195	GLU
1	B	282	TYR
2	A	22	LEU
2	A	139	LYS
2	A	178	GLN
1	B	104	ILE

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	B	166/196 (85%)	136 (82%)	30 (18%)	1 4
2	A	214/216 (99%)	186 (87%)	28 (13%)	4 12
All	All	380/412 (92%)	322 (85%)	58 (15%)	2 8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	ARG

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Mol	Chain	Res	Type
1	B	87	LEU
1	B	104	ILE
1	B	106	ILE
1	B	112	LEU
1	B	115	VAL
1	B	118	ASP
1	B	137	VAL
1	B	156	ASN
1	B	167	MET
1	B	173	THR
1	B	178	LEU
1	B	196	THR
1	B	200	ASP
1	B	201	PHE
1	B	223	ILE
1	B	226	ASP
1	B	227	PHE
1	B	232	TYR
1	B	233	LEU
1	B	235	TYR
1	B	254	THR
1	B	255	ASN
1	B	258	LEU
1	B	264	LEU
1	B	274	ASP
1	B	276	LYS
1	B	281	GLN
1	B	286	LEU
1	B	291	ASN
2	A	12	THR
2	A	36	LEU
2	A	38	THR
2	A	49	THR
2	A	51	ASP
2	A	52	LYS
2	A	62	SER
2	A	63	VAL
2	A	73	ARG
2	A	75	VAL
2	A	86	LEU
2	A	89	LEU
2	A	91	THR

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Mol	Chain	Res	Type
2	A	92	THR
2	A	113	LEU
2	A	116	ILE
2	A	127	THR
2	A	134	ASP
2	A	136	LEU
2	A	151	GLN
2	A	157	LYS
2	A	168	LEU
2	A	178	GLN
2	A	190	ILE
2	A	193	ILE
2	A	205	GLU
2	A	213	LEU
2	A	231	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	HIS
1	B	255	ASN
1	B	281	GLN
1	B	291	ASN
2	A	47	ASN
2	A	131	ASN
2	A	155	GLN
2	A	192	ASN
2	A	212	HIS
2	A	230	HIS

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	189/217 (87%)	-0.00	6 (3%)	47 44	55, 111, 184, 216	0
2	A	236/238 (99%)	-0.11	1 (0%)	92 92	50, 88, 131, 186	0
All	All	425/455 (93%)	-0.06	7 (1%)	72 71	50, 96, 174, 216	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	PHE	3.8
2	A	49	THR	3.6
1	B	235	TYR	3.3
1	B	246	TYR	2.9
1	B	78	GLY	2.7
1	B	150	ASN	2.4
1	B	232	TYR	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. 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
3	MG	B	301	1/1	0.74	0.38	74,74,74,74	1
3	MG	B	302	1/1	0.91	0.23	96,96,96,96	0
4	ZN	A	301	1/1	0.98	0.22	65,65,65,65	0
4	ZN	A	302	1/1	0.99	0.12	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.