Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NVN
Title	:	Molecular mechanism of guidance cue recognition
Authors	:	Liu, H.; Juo, Z.; Shim, A.; Focia, P.; Chen, X.; Garcia, C.; He, X.
Deposited on	:	2010-07-08
Resolution	:	2.26 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

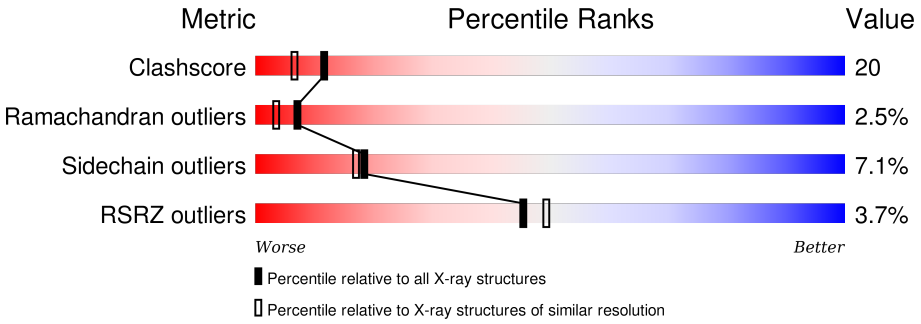
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.26 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	389	2% 64% 29% 5%
2	B	476	5% 63% 32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7296 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 EVM139.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3052	1943	508	589	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	PRO	-	EXPRESSION TAG	UNP Q8JL80
A	13	GLY	-	EXPRESSION TAG	UNP Q8JL80
A	14	THR	-	EXPRESSION TAG	UNP Q8JL80
A	15	SER	-	EXPRESSION TAG	UNP Q8JL80

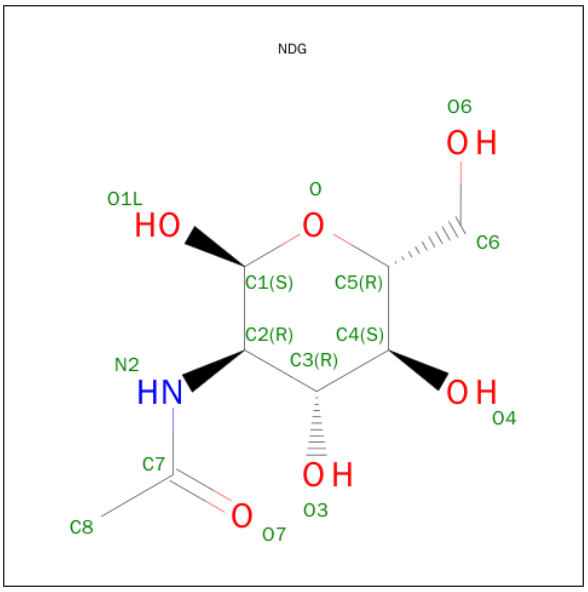
- Molecule 2 is a protein called Plexin-C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	474	Total	C	N	O	S	0	0	0
			3622	2262	645	694	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	508	GLY	-	EXPRESSION TAG	UNP O60486
B	509	ALA	-	EXPRESSION TAG	UNP O60486
B	510	PRO	-	EXPRESSION TAG	UNP O60486

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

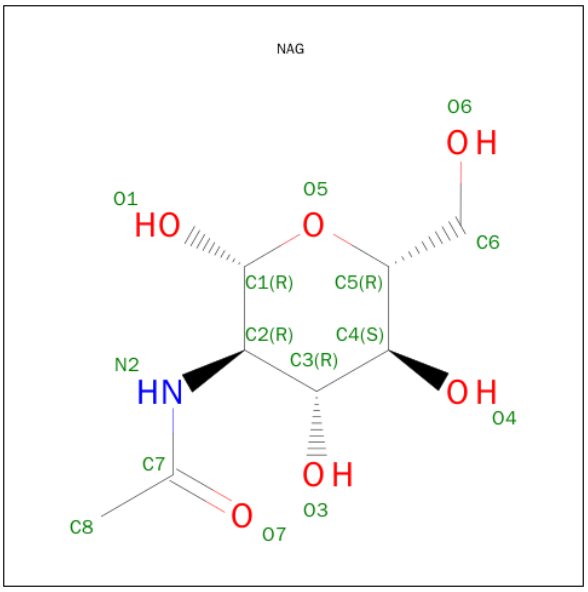


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

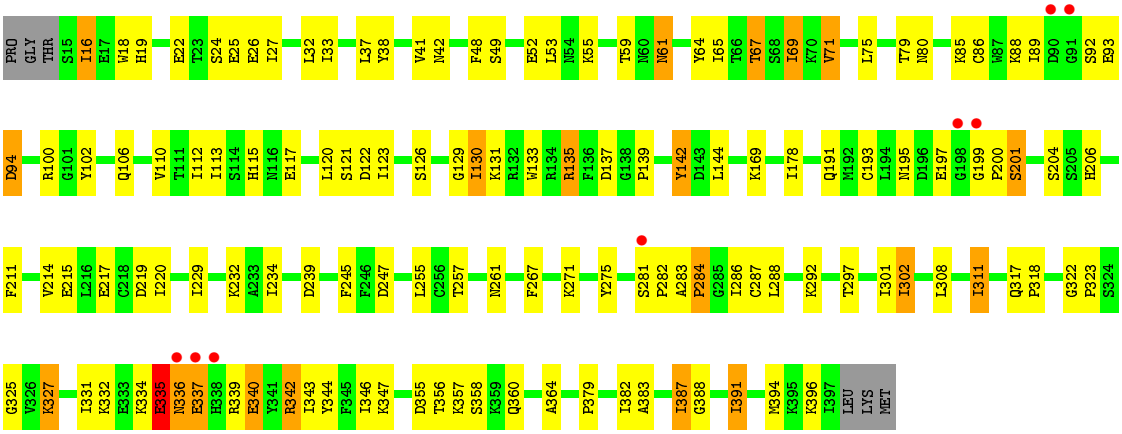
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 267 267	0	0
6	B	242	Total O 242 242	0	0

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 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.

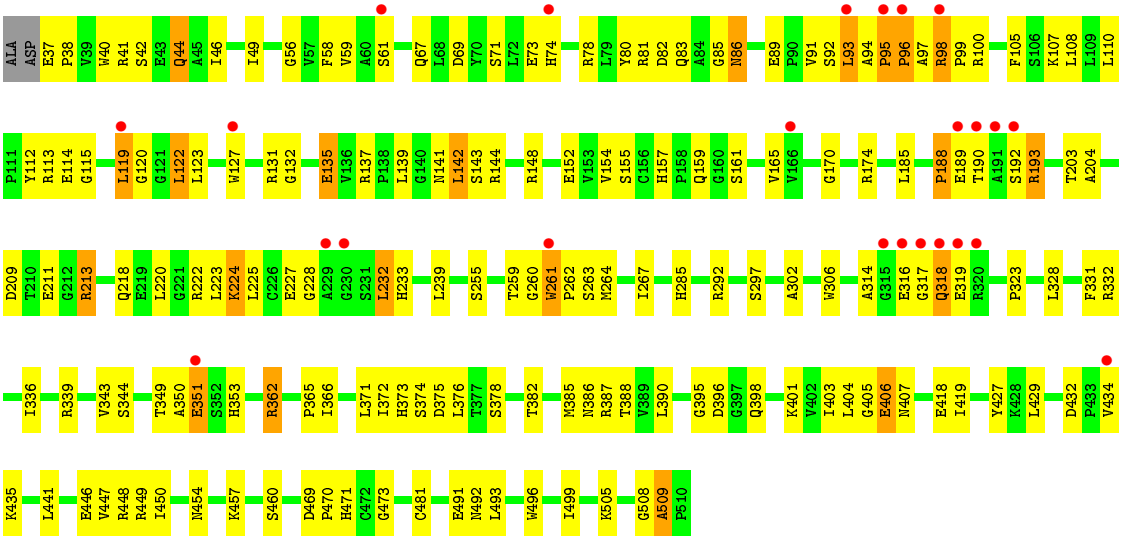
- Molecule 1: EVM139

Chain A:



- Molecule 2: Plexin-C1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	95.75Å 133.49Å 172.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.53 – 2.26 43.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.53-2.26) 99.0 (43.53-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.276 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	1 of 73704 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, NAG, NDG

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	0.56	1/3123 (0.0%)	0.65	0/4231
2	B	0.39	1/3706 (0.0%)	0.64	0/5040
All	All	0.48	2/6829 (0.0%)	0.64	0/9271

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	SER	CB-OG	-22.24	1.13	1.42
2	B	86	ASN	CB-CG	-6.49	1.36	1.51

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	A	3052	0	2995	135	0
2	B	3622	0	3499	141	0
3	A	14	0	13	0	0
3	B	28	0	26	1	0
4	B	1	0	0	0	0
5	B	70	0	65	4	0
6	A	267	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	242	0	0	15	0
All	All	7296	0	6598	271	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 20.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HE3	1:A:234:ILE:HD11	1.33	1.09
1:A:229:ILE:HD11	1:A:247:ASP:HB2	1.25	1.07
1:A:334:LYS:HE3	1:A:355:ASP:OD2	1.57	1.04
1:A:391:ILE:HD13	1:A:391:ILE:H	1.23	1.03
1:A:281:SER:HB2	1:A:282:PRO:HD3	1.44	0.99
2:B:91:VAL:HG12	2:B:92:SER:H	1.29	0.98
1:A:110:VAL:HG13	1:A:123:ILE:HD11	1.46	0.98
1:A:199:GLY:HA3	1:A:204:SER:O	1.67	0.95
1:A:75:LEU:HD11	1:A:86:CYS:HB3	1.52	0.92
1:A:100:ARG:HH21	2:B:220:LEU:HD12	1.38	0.88
1:A:100:ARG:NH2	2:B:220:LEU:HD12	1.91	0.85
2:B:49:ILE:HD13	2:B:59:VAL:HG22	1.58	0.85
2:B:261:TRP:HD1	2:B:262:PRO:HD2	1.41	0.85
1:A:340:GLU:HG3	1:A:356:THR:OG1	1.76	0.84
1:A:229:ILE:HD11	1:A:247:ASP:CB	2.08	0.84
2:B:174:ARG:NH2	2:B:211:GLU:HB2	1.93	0.82
2:B:204:ALA:HB2	2:B:225:LEU:HG	1.61	0.81
1:A:88:LYS:HB2	1:A:92:SER:HB2	1.62	0.81
2:B:174:ARG:HH22	2:B:211:GLU:HB2	1.45	0.79
2:B:41:ARG:HG2	2:B:446:GLU:HG2	1.65	0.78
2:B:98:ARG:HH11	2:B:98:ARG:HG3	1.48	0.77
1:A:41:VAL:HG22	1:A:42:ASN:H	1.52	0.74
1:A:335:GLU:HG3	1:A:335:GLU:O	1.87	0.74
1:A:340:GLU:HG2	1:A:357:LYS:HB2	1.70	0.73
1:A:391:ILE:CD1	1:A:391:ILE:H	2.01	0.72
1:A:323:PRO:HG2	1:A:347:LYS:HD2	1.71	0.72
2:B:499:ILE:HG12	6:B:642:HOH:O	1.90	0.72
1:A:27:ILE:HD11	1:A:383:ALA:C	2.10	0.72
1:A:239:ASP:HB3	1:A:261:ASN:ND2	2.06	0.71
1:A:217:GLU:HB2	1:A:311:ILE:CD1	2.21	0.70
1:A:27:ILE:HD11	1:A:383:ALA:O	1.91	0.70
2:B:259:THR:HG21	5:B:5:NAG:O7	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:LEU:HD21	2:B:390:LEU:HD13	1.75	0.69
2:B:91:VAL:HG12	2:B:92:SER:N	2.07	0.68
1:A:135:ARG:NH1	1:A:144:LEU:HD22	2.09	0.68
2:B:86:ASN:OD1	6:B:563:HOH:O	2.11	0.68
2:B:157:HIS:HB3	2:B:159:GLN:HE21	1.59	0.68
1:A:41:VAL:HG22	1:A:42:ASN:N	2.09	0.67
2:B:98:ARG:NH1	2:B:98:ARG:HG3	2.10	0.67
1:A:331:ILE:HD12	1:A:343:ILE:HG12	1.76	0.67
1:A:360:GLN:HB3	6:A:533:HOH:O	1.93	0.66
2:B:255:SER:HB3	5:B:5:NAG:O6	1.94	0.66
2:B:302:ALA:HB2	6:B:697:HOH:O	1.96	0.66
2:B:89:GLU:HB3	2:B:105:PHE:CE2	2.31	0.66
1:A:16:ILE:HD11	1:A:388:GLY:HA3	1.78	0.66
2:B:448:ARG:HB2	2:B:450:ILE:HD11	1.76	0.65
1:A:142:TYR:HB2	6:A:415:HOH:O	1.95	0.65
2:B:157:HIS:HB3	2:B:159:GLN:NE2	2.11	0.65
1:A:364:ALA:HB2	1:A:394:MET:HG2	1.78	0.65
2:B:188:PRO:HG2	2:B:189:GLU:H	1.61	0.65
2:B:107:LYS:HB2	2:B:154:VAL:HG11	1.78	0.65
1:A:67:THR:HG21	1:A:102:TYR:O	1.97	0.64
2:B:82:ASP:OD1	2:B:83:GLN:HG3	1.98	0.64
2:B:398:GLN:HG2	2:B:418:GLU:HG2	1.79	0.64
1:A:217:GLU:HB2	1:A:311:ILE:HD11	1.80	0.64
2:B:99:PRO:HG2	2:B:314:ALA:HB2	1.80	0.64
2:B:450:ILE:N	2:B:450:ILE:HD12	2.12	0.64
1:A:85:LYS:HE2	6:A:661:HOH:O	1.97	0.64
2:B:89:GLU:HB3	2:B:105:PHE:HE2	1.64	0.63
2:B:406:GLU:HG3	2:B:407:ASN:H	1.63	0.63
1:A:100:ARG:HH21	2:B:220:LEU:CD1	2.12	0.63
1:A:232:LYS:HE3	1:A:234:ILE:CD1	2.22	0.62
1:A:33:ILE:HD13	1:A:38:TYR:CD2	2.34	0.62
2:B:97:ALA:HB1	2:B:99:PRO:HD2	1.82	0.61
1:A:281:SER:CB	1:A:282:PRO:HD3	2.27	0.61
2:B:388:THR:HB	2:B:404:LEU:HD12	1.81	0.61
1:A:130:ILE:HG23	1:A:130:ILE:O	1.99	0.60
2:B:93:LEU:HD21	2:B:105:PHE:CE2	2.36	0.60
1:A:110:VAL:CG1	1:A:123:ILE:HD11	2.28	0.60
2:B:93:LEU:O	2:B:95:PRO:HD3	2.02	0.60
1:A:89:ILE:HG22	6:A:575:HOH:O	2.01	0.60
1:A:199:GLY:CA	1:A:204:SER:O	2.48	0.59
1:A:396:LYS:HG2	6:A:533:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HD21	1:A:85:LYS:HB3	1.67	0.59
1:A:93:GLU:HB2	6:A:589:HOH:O	2.02	0.59
2:B:375:ASP:OD1	2:B:395:GLY:HA3	2.03	0.59
2:B:141:ASN:HB3	2:B:144:ARG:HD2	1.84	0.58
1:A:229:ILE:HD11	1:A:247:ASP:N	2.19	0.58
1:A:284:PRO:HB3	1:A:302:ILE:HG12	1.85	0.58
2:B:115:GLY:HA2	6:B:544:HOH:O	2.04	0.58
2:B:373:HIS:HB3	2:B:376:LEU:HG	1.85	0.58
1:A:25:GLU:HB3	1:A:41:VAL:HG21	1.86	0.57
1:A:215:GLU:HB3	1:A:311:ILE:HG12	1.84	0.57
2:B:261:TRP:CZ3	2:B:362:ARG:NE	2.73	0.57
2:B:223:LEU:HD22	2:B:267:ILE:HD11	1.86	0.57
1:A:33:ILE:HD12	1:A:33:ILE:N	2.19	0.57
1:A:229:ILE:CD1	1:A:247:ASP:HB2	2.17	0.57
2:B:222:ARG:HG3	2:B:224:LYS:HE2	1.87	0.57
1:A:93:GLU:HG3	6:A:514:HOH:O	2.05	0.57
2:B:508:GLY:O	2:B:509:ALA:C	2.44	0.56
2:B:113:ARG:HD3	2:B:122:LEU:HD22	1.86	0.56
1:A:217:GLU:HB2	1:A:311:ILE:HD12	1.87	0.56
1:A:32:LEU:C	1:A:33:ILE:HD12	2.26	0.56
2:B:387:ARG:HH21	2:B:405:GLY:HA2	1.71	0.56
2:B:297:SER:HG	2:B:306:TRP:HE1	1.52	0.56
1:A:93:GLU:O	1:A:94:ASP:HB3	2.06	0.56
1:A:301:ILE:HD11	6:A:594:HOH:O	2.06	0.56
2:B:285:HIS:HD2	2:B:372:ILE:HD11	1.71	0.55
2:B:78:ARG:HD3	2:B:80:TYR:CE1	2.41	0.55
2:B:99:PRO:HG2	2:B:314:ALA:CB	2.37	0.55
2:B:190:THR:HA	2:B:193:ARG:HB2	1.86	0.55
1:A:193:CYS:HB3	6:A:447:HOH:O	2.07	0.55
2:B:218:GLN:HG2	6:B:712:HOH:O	2.06	0.54
1:A:121:SER:OG	1:A:123:ILE:HD13	2.08	0.54
1:A:33:ILE:HD13	1:A:38:TYR:CE2	2.43	0.54
1:A:358:SER:HB2	1:A:360:GLN:HE21	1.72	0.54
1:A:387:ILE:H	1:A:387:ILE:HD13	1.73	0.54
2:B:93:LEU:HD22	2:B:93:LEU:N	2.23	0.53
2:B:261:TRP:CD1	2:B:262:PRO:HD2	2.33	0.53
2:B:264:MET:CE	2:B:336:ILE:HG21	2.39	0.53
1:A:75:LEU:HD11	1:A:86:CYS:CB	2.34	0.53
2:B:351:GLU:N	2:B:351:GLU:OE1	2.38	0.53
1:A:144:LEU:HA	1:A:206:HIS:O	2.09	0.53
2:B:119:LEU:HD22	2:B:120:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:HB3	1:A:286:ILE:HD12	1.90	0.53
2:B:331:PHE:CZ	2:B:365:PRO:HB3	2.43	0.53
2:B:154:VAL:CG1	2:B:155:SER:N	2.71	0.53
2:B:81:ARG:HD3	6:B:606:HOH:O	2.08	0.53
2:B:225:LEU:CD2	2:B:232:LEU:HD22	2.39	0.53
1:A:297:THR:HG23	6:A:557:HOH:O	2.09	0.53
1:A:69:ILE:H	1:A:69:ILE:HD13	1.74	0.53
1:A:283:ALA:HB3	1:A:286:ILE:CD1	2.39	0.53
2:B:225:LEU:HD23	2:B:232:LEU:HD22	1.91	0.52
2:B:213:ARG:HG3	2:B:213:ARG:O	2.09	0.52
1:A:360:GLN:OE1	1:A:396:LYS:HE3	2.09	0.52
1:A:110:VAL:HG22	1:A:123:ILE:HG13	1.91	0.52
1:A:49:SER:O	1:A:52:GLU:HG2	2.09	0.52
2:B:98:ARG:N	2:B:99:PRO:CD	2.73	0.52
2:B:135:GLU:HG3	2:B:137:ARG:NH2	2.24	0.52
1:A:16:ILE:C	1:A:16:ILE:HD13	2.30	0.52
2:B:91:VAL:CG1	2:B:92:SER:H	2.12	0.51
2:B:378:SER:OG	2:B:429:LEU:HG	2.10	0.51
1:A:26:GLU:O	1:A:41:VAL:HG23	2.11	0.51
2:B:261:TRP:HD1	2:B:262:PRO:CD	2.19	0.51
1:A:211:PHE:O	1:A:302:ILE:CD1	2.59	0.51
1:A:275:TYR:CE1	1:A:301:ILE:HD12	2.46	0.51
2:B:264:MET:HE2	2:B:336:ILE:HG21	1.92	0.51
1:A:211:PHE:O	1:A:302:ILE:HD11	2.11	0.51
2:B:161:SER:HB3	2:B:233:HIS:ND1	2.25	0.51
1:A:80:ASN:ND2	1:A:85:LYS:HB3	2.26	0.51
2:B:454:ASN:O	2:B:457:LYS:HG2	2.11	0.51
2:B:174:ARG:NH2	2:B:209:ASP:OD1	2.44	0.51
1:A:16:ILE:HG23	1:A:16:ILE:O	2.10	0.50
2:B:78:ARG:HD3	2:B:80:TYR:CZ	2.46	0.50
1:A:229:ILE:HD12	1:A:229:ILE:N	2.27	0.50
1:A:229:ILE:CD1	1:A:247:ASP:N	2.74	0.50
1:A:65:ILE:N	1:A:65:ILE:HD12	2.26	0.50
2:B:74:HIS:HA	6:B:520:HOH:O	2.12	0.50
1:A:25:GLU:OE1	1:A:41:VAL:HG21	2.11	0.49
2:B:260:GLY:O	2:B:292:ARG:HG2	2.12	0.49
1:A:123:ILE:HD12	1:A:123:ILE:N	2.26	0.49
1:A:297:THR:O	1:A:301:ILE:HG12	2.12	0.49
2:B:193:ARG:HG3	6:B:614:HOH:O	2.12	0.49
2:B:189:GLU:HA	6:B:693:HOH:O	2.12	0.49
2:B:108:LEU:CD2	2:B:110:LEU:HG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:O	1:A:79:THR:HG23	2.12	0.49
1:A:201:SER:HB2	2:B:152:GLU:HB2	1.95	0.49
1:A:113:ILE:HG13	6:A:652:HOH:O	2.13	0.49
1:A:331:ILE:CD1	1:A:343:ILE:HG23	2.43	0.48
2:B:505:LYS:NZ	2:B:505:LYS:HB3	2.27	0.48
2:B:323:PRO:HA	2:B:374:SER:HB3	1.95	0.48
2:B:170:GLY:HA3	6:B:579:HOH:O	2.13	0.48
1:A:302:ILE:HD13	1:A:302:ILE:O	2.13	0.48
1:A:219:ASP:C	1:A:220:ILE:HD12	2.33	0.48
2:B:165:VAL:HG21	2:B:239:LEU:HD13	1.94	0.48
1:A:169:LYS:HE3	1:A:287:CYS:SG	2.53	0.48
1:A:117:GLU:HB3	1:A:139:PRO:HG2	1.95	0.48
2:B:112:TYR:CD1	2:B:113:ARG:HG3	2.49	0.48
2:B:427:TYR:HB3	6:B:522:HOH:O	2.13	0.48
1:A:214:VAL:HG23	1:A:267:PHE:CZ	2.49	0.48
2:B:432:ASP:HB3	2:B:435:LYS:O	2.13	0.48
1:A:387:ILE:O	1:A:387:ILE:HG12	2.14	0.47
2:B:434:VAL:HG12	2:B:435:LYS:HD2	1.97	0.47
2:B:401:LYS:NZ	2:B:471:HIS:HD2	2.13	0.47
1:A:257:THR:HG21	1:A:318:PRO:HD2	1.96	0.47
2:B:127:TRP:O	2:B:132:GLY:HA2	2.13	0.47
2:B:73:GLU:HG3	2:B:74:HIS:CD2	2.49	0.47
1:A:178:ILE:HD12	1:A:178:ILE:N	2.30	0.47
2:B:131:ARG:HD3	6:B:668:HOH:O	2.15	0.47
1:A:41:VAL:CG2	1:A:42:ASN:H	2.24	0.47
2:B:49:ILE:CD1	2:B:59:VAL:HG22	2.37	0.46
1:A:69:ILE:N	1:A:69:ILE:HD13	2.29	0.46
1:A:325:GLY:HA3	1:A:347:LYS:HE3	1.97	0.46
2:B:473:GLY:HA3	2:B:496:TRP:CE2	2.51	0.46
1:A:100:ARG:HD2	6:A:416:HOH:O	2.16	0.46
1:A:75:LEU:CD1	1:A:86:CYS:HB3	2.35	0.46
2:B:93:LEU:H	2:B:93:LEU:HD22	1.81	0.46
2:B:192:SER:O	2:B:193:ARG:C	2.54	0.46
1:A:382:ILE:HD12	1:A:382:ILE:N	2.31	0.45
1:A:335:GLU:O	1:A:337:GLU:N	2.49	0.45
2:B:94:ALA:O	2:B:96:PRO:HD3	2.16	0.45
1:A:311:ILE:HG23	1:A:311:ILE:O	2.16	0.45
1:A:344:TYR:CE2	1:A:391:ILE:HG21	2.52	0.45
2:B:107:LYS:CB	2:B:154:VAL:HG11	2.44	0.45
1:A:214:VAL:HG22	1:A:308:LEU:HD12	1.99	0.45
2:B:469:ASP:HA	2:B:470:PRO:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:HB3	1:A:41:VAL:CG2	2.47	0.45
2:B:344:SER:HB2	2:B:349:THR:OG1	2.16	0.45
1:A:379:PRO:HG3	1:A:391:ILE:HG23	1.98	0.45
1:A:16:ILE:HD12	1:A:18:TRP:CD1	2.51	0.45
1:A:340:GLU:HA	1:A:340:GLU:OE1	2.17	0.45
2:B:157:HIS:CG	2:B:185:LEU:HD12	2.52	0.45
2:B:97:ALA:CB	2:B:100:ARG:HH11	2.30	0.45
1:A:302:ILE:HD12	6:A:401:HOH:O	2.17	0.45
1:A:327:LYS:HG2	1:A:346:ILE:HD12	1.98	0.45
2:B:441:LEU:HB3	2:B:450:ILE:HD13	1.99	0.45
1:A:19:HIS:HB2	1:A:387:ILE:CD1	2.47	0.45
1:A:195:ASN:HD22	1:A:195:ASN:N	2.15	0.44
1:A:232:LYS:CE	1:A:234:ILE:HD11	2.22	0.44
2:B:108:LEU:HD23	2:B:110:LEU:HG	1.98	0.44
1:A:334:LYS:HE3	1:A:355:ASP:CG	2.35	0.44
1:A:199:GLY:O	2:B:213:ARG:NH2	2.51	0.44
2:B:49:ILE:HD12	2:B:58:PHE:O	2.17	0.44
2:B:350:ALA:HB3	2:B:351:GLU:OE1	2.17	0.44
2:B:339:ARG:HG3	2:B:339:ARG:HH11	1.82	0.44
1:A:122:ASP:O	1:A:131:LYS:HE2	2.18	0.44
2:B:40:TRP:CZ3	2:B:42:SER:HB2	2.53	0.44
1:A:41:VAL:CG2	1:A:42:ASN:N	2.78	0.44
2:B:388:THR:CB	2:B:404:LEU:HD12	2.47	0.44
2:B:372:ILE:HD12	2:B:372:ILE:N	2.33	0.44
2:B:46:ILE:HD13	2:B:447:VAL:CG2	2.47	0.44
1:A:288:LEU:HB3	1:A:292:LYS:HB2	2.00	0.44
1:A:16:ILE:HD11	1:A:388:GLY:CA	2.44	0.44
2:B:203:THR:HG21	2:B:222:ARG:HD3	1.99	0.44
2:B:419:ILE:HG23	2:B:448:ARG:HH21	1.82	0.44
2:B:317:GLY:O	2:B:318:GLN:HB2	2.18	0.44
2:B:141:ASN:OD1	2:B:143:SER:N	2.45	0.43
1:A:115:HIS:HD2	6:A:585:HOH:O	2.00	0.43
2:B:255:SER:HB3	5:B:5:NAG:HO6	1.83	0.43
2:B:450:ILE:CD1	2:B:450:ILE:N	2.81	0.43
2:B:492:ASN:ND2	2:B:493:LEU:HG	2.33	0.43
2:B:499:ILE:HD11	6:B:686:HOH:O	2.18	0.43
1:A:112:ILE:HG13	1:A:121:SER:HB2	2.00	0.43
2:B:403:ILE:HD13	2:B:469:ASP:HA	1.99	0.43
2:B:114:GLU:HG3	6:B:607:HOH:O	2.18	0.43
2:B:38:PRO:HD2	2:B:449:ARG:HB3	2.01	0.43
2:B:38:PRO:HB3	2:B:71:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:OD2	1:A:142:TYR:HA	2.18	0.42
2:B:85:GLY:O	2:B:86:ASN:C	2.57	0.42
1:A:129:GLY:O	1:A:130:ILE:HG22	2.19	0.42
2:B:123:LEU:HB2	2:B:139:LEU:HD13	2.02	0.42
1:A:331:ILE:HD13	1:A:343:ILE:HG23	2.01	0.42
1:A:120:LEU:HB3	1:A:133:TRP:CZ2	2.54	0.42
2:B:332:ARG:NH2	3:B:7:NDG:H8C3	2.35	0.42
2:B:328:LEU:HB3	2:B:371:LEU:HB3	2.00	0.42
1:A:332:LYS:HE3	6:A:455:HOH:O	2.20	0.42
1:A:311:ILE:CG2	1:A:311:ILE:O	2.67	0.42
2:B:157:HIS:CD2	2:B:185:LEU:HD12	2.55	0.42
2:B:343:VAL:HG23	6:B:624:HOH:O	2.20	0.42
1:A:135:ARG:NH1	1:A:142:TYR:O	2.50	0.41
2:B:86:ASN:OD1	5:B:1:NAG:O5	2.35	0.41
2:B:441:LEU:CB	2:B:450:ILE:HD13	2.50	0.41
2:B:227:GLU:HG2	2:B:228:GLY:N	2.35	0.41
1:A:93:GLU:HA	6:A:472:HOH:O	2.19	0.41
1:A:19:HIS:HB2	1:A:387:ILE:HD11	2.01	0.41
1:A:106:GLN:HB2	6:A:618:HOH:O	2.20	0.41
2:B:37:GLU:HA	2:B:38:PRO:HD3	1.87	0.41
2:B:44:GLN:HB2	2:B:44:GLN:HE21	1.65	0.41
1:A:88:LYS:HB2	1:A:92:SER:CB	2.42	0.41
2:B:505:LYS:HZ2	2:B:505:LYS:HB3	1.86	0.41
2:B:401:LYS:HZ1	2:B:471:HIS:HD2	1.69	0.41
2:B:403:ILE:HD13	2:B:470:PRO:HD2	2.01	0.41
2:B:385:MET:HA	2:B:385:MET:CE	2.51	0.41
1:A:282:PRO:HD2	6:A:482:HOH:O	2.21	0.40
2:B:141:ASN:HB3	2:B:144:ARG:CD	2.51	0.40
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.86	0.40
1:A:281:SER:HB2	1:A:282:PRO:CD	2.33	0.40
2:B:127:TRP:CZ3	2:B:135:GLU:OE2	2.75	0.40
1:A:37:LEU:HB3	1:A:48:PHE:HB3	2.02	0.40
2:B:67:GLN:HB2	2:B:142:LEU:HD22	2.03	0.40
2:B:69:ASP:OD2	2:B:71:SER:HB2	2.22	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	381/389 (98%)	344 (90%)	28 (7%)	9 (2%)	7	3
2	B	472/476 (99%)	424 (90%)	36 (8%)	12 (2%)	7	3
All	All	853/865 (99%)	768 (90%)	64 (8%)	21 (2%)	7	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	GLU
1	A	336	ASN
2	B	318	GLN
1	A	71	VAL
1	A	200	PRO
1	A	337	GLU
2	B	188	PRO
2	B	319	GLU
2	B	353	HIS
1	A	130	ILE
2	B	96	PRO
2	B	193	ARG
2	B	386	ASN
2	B	406	GLU
1	A	61	ASN
1	A	94	ASP
1	A	322	GLY
2	B	366	ILE
2	B	509	ALA
2	B	95	PRO
2	B	56	GLY

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	343/349 (98%)	313 (91%)	30 (9%)	13 11
2	B	389/390 (100%)	367 (94%)	22 (6%)	25 26
All	All	732/739 (99%)	680 (93%)	52 (7%)	18 17

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	22	GLU
1	A	24	SER
1	A	53	LEU
1	A	55	LYS
1	A	59	THR
1	A	61	ASN
1	A	67	THR
1	A	69	ILE
1	A	71	VAL
1	A	126	SER
1	A	135	ARG
1	A	142	TYR
1	A	191	GLN
1	A	197	GLU
1	A	245	PHE
1	A	255	LEU
1	A	271	LYS
1	A	284	PRO
1	A	302	ILE
1	A	311	ILE
1	A	317	GLN
1	A	327	LYS
1	A	335	GLU
1	A	336	ASN
1	A	339	ARG
1	A	340	GLU

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Mol	Chain	Res	Type
1	A	342	ARG
1	A	387	ILE
1	A	391	ILE
2	B	44	GLN
2	B	61	SER
2	B	93	LEU
2	B	98	ARG
2	B	119	LEU
2	B	122	LEU
2	B	135	GLU
2	B	142	LEU
2	B	148	ARG
2	B	213	ARG
2	B	224	LYS
2	B	232	LEU
2	B	261	TRP
2	B	263	SER
2	B	316	GLU
2	B	351	GLU
2	B	362	ARG
2	B	382	THR
2	B	396	ASP
2	B	460	SER
2	B	481	CYS
2	B	491	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	81	ASN
1	A	107	ASN
1	A	195	ASN
1	A	317	GLN
1	A	336	ASN
1	A	349	ASN
1	A	360	GLN
1	A	365	GLN
2	B	44	GLN
2	B	67	GLN
2	B	159	GLN
2	B	285	HIS

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Mol	Chain	Res	Type
2	B	471	HIS
2	B	479	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	NDG	A	1	-	14,14,15	0.68	0	15,19,21	0.93	1 (6%)
5	NAG	B	1	2	14,14,15	1.12	1 (7%)	15,19,21	1.00	1 (6%)
3	NDG	B	2	-	14,14,15	0.62	0	15,19,21	0.71	0
5	NAG	B	3	2	14,14,15	0.53	0	15,19,21	0.96	1 (6%)
5	NAG	B	4	-	14,14,15	0.65	0	15,19,21	1.10	2 (13%)
5	NAG	B	5	2	14,14,15	0.49	0	15,19,21	0.89	1 (6%)
5	NAG	B	6	2	14,14,15	0.48	0	15,19,21	0.70	0
3	NDG	B	7	-	14,14,15	0.75	0	15,19,21	0.59	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
3	NDG	A	1	-	-	1/6/23/26	0/1/1/1
5	NAG	B	1	2	-	0/6/23/26	0/1/1/1
3	NDG	B	2	-	-	0/6/23/26	0/1/1/1
5	NAG	B	3	2	-	0/6/23/26	0/1/1/1
5	NAG	B	4	-	-	0/6/23/26	0/1/1/1
5	NAG	B	5	2	-	0/6/23/26	0/1/1/1
5	NAG	B	6	2	-	0/6/23/26	0/1/1/1
3	NDG	B	7	-	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	NAG	C1-C2	-3.42	1.47	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3	NAG	C2-N2-C7	-2.88	119.34	123.04
5	B	1	NAG	C2-N2-C7	-2.73	119.53	123.04
5	B	4	NAG	C2-N2-C7	-2.66	119.62	123.04
5	B	5	NAG	C2-N2-C7	-2.32	120.05	123.04
3	A	1	NDG	C4-C3-C2	2.03	114.39	111.23
5	B	4	NAG	C3-C4-C5	2.71	114.91	110.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NDG	O7-C7-N2-C2
3	B	7	NDG	C8-C7-N2-C2
3	B	7	NDG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	1	0
5	B	5	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7	NDG	1	0

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	383/389 (98%)	0.01	8 (2%) 67 71	14, 37, 89, 135	0
2	B	474/476 (99%)	0.21	24 (5%) 32 35	15, 42, 102, 147	0
All	All	857/865 (99%)	0.12	32 (3%) 45 49	14, 40, 98, 147	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	315	GLY	9.6
2	B	318	GLN	8.7
2	B	229	ALA	7.4
1	A	281	SER	6.4
2	B	119	LEU	5.4
2	B	316	GLU	5.1
2	B	230	GLY	4.9
2	B	190	THR	4.8
1	A	199	GLY	4.6
2	B	319	GLU	4.5
2	B	317	GLY	4.5
1	A	337	GLU	3.9
2	B	320	ARG	3.7
2	B	93	LEU	3.6
1	A	336	ASN	3.3
2	B	192	SER	3.1
1	A	198	GLY	2.9
2	B	98	ARG	2.8
2	B	261	TRP	2.7
1	A	91	GLY	2.7
2	B	191	ALA	2.6
2	B	96	PRO	2.6
2	B	166	VAL	2.5
2	B	61	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	351	GLU	2.4
2	B	189	GLU	2.4
2	B	74	HIS	2.3
2	B	127	TRP	2.2
1	A	338	HIS	2.1
2	B	434	VAL	2.1
1	A	90	ASP	2.1
2	B	95	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NDG	A	1	14/15	0.64	0.35	0.14	146,146,146,146	0
5	NAG	B	4	14/15	0.88	0.14	-0.04	46,52,53,54	0
4	CA	B	801	1/1	0.96	0.13	-1.21	62,62,62,62	0
5	NAG	B	6	14/15	0.48	0.58	-	192,195,198,199	0
5	NAG	B	3	14/15	0.81	0.17	-	113,113,114,114	0
3	NDG	B	7	14/15	0.22	0.61	-	170,170,170,170	0
5	NAG	B	1	14/15	0.65	0.26	-	166,166,166,166	0
5	NAG	B	5	14/15	0.61	0.24	-	107,108,109,109	0
3	NDG	B	2	14/15	0.71	0.37	-	136,136,136,136	0

6.5 Other polymers (i)

There are no such residues in this entry.