



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:11 AM GMT

PDB ID : 2G1O
Title : Ketopiperazine-Based Renin Inhibitors: Optimization of the "C" Ring
Authors : Holsworth, D.D.; Zhanga, E.
Deposited on : 2006-02-14
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

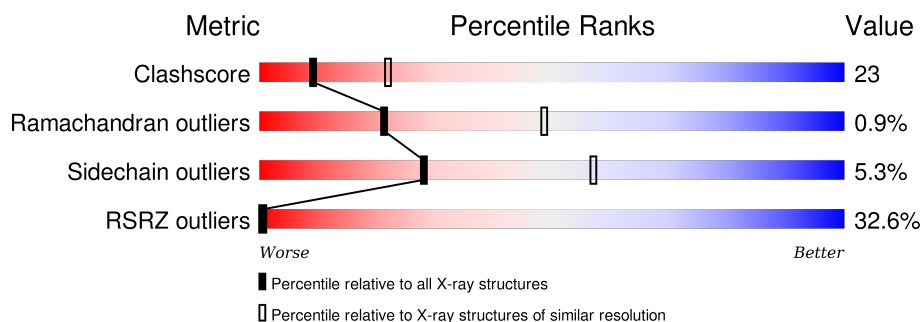
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	986	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5498 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 Renin.

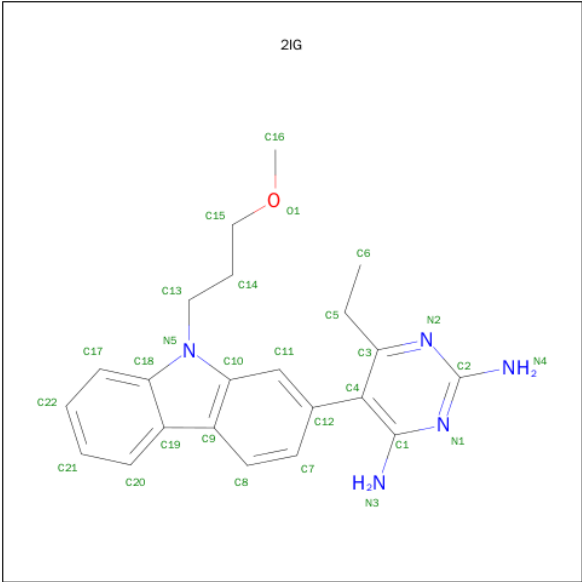
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2572	1642	416	500	14			
1	B	333	Total	C	N	O	S	0	0	0
			2572	1642	416	500	14			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is 6-ETHYL-5-[9-(3-METHOXYPROPYL)-9H-CARBAZOL-2-YL]PYRIMIDIN E-2,4-DIAMINE (three-letter code: 2IG) (formula: $C_{22}H_{25}N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	5	1		
3	B	1	Total	C	N	O	0	0
			28	22	5	1		

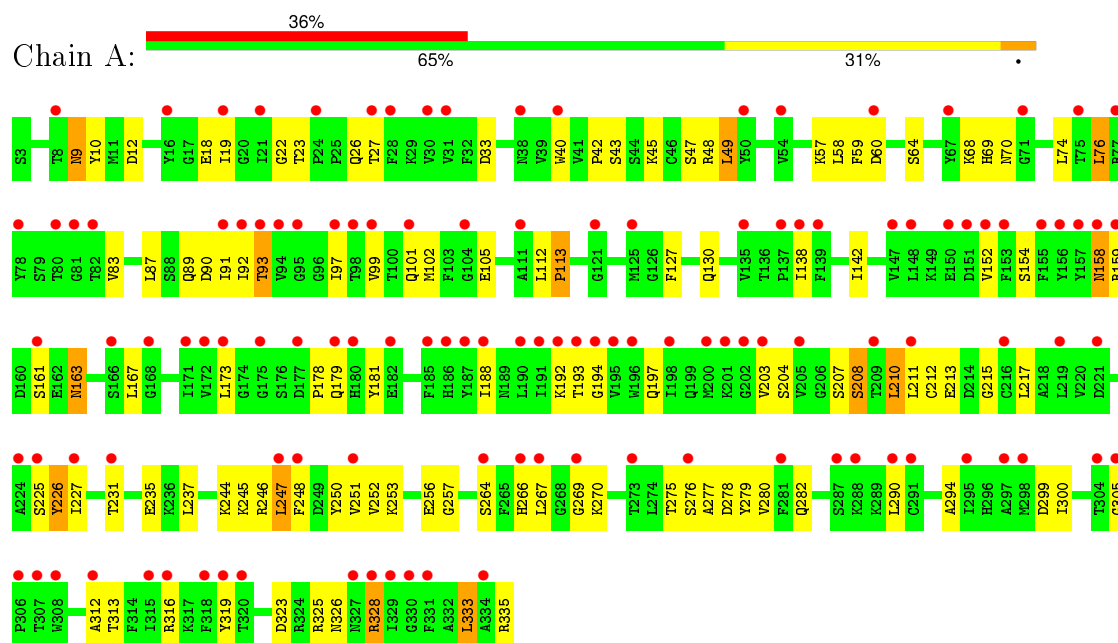
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	158	Total	O	0	0
			158	158		
4	B	112	Total	O	0	0
			112	112		

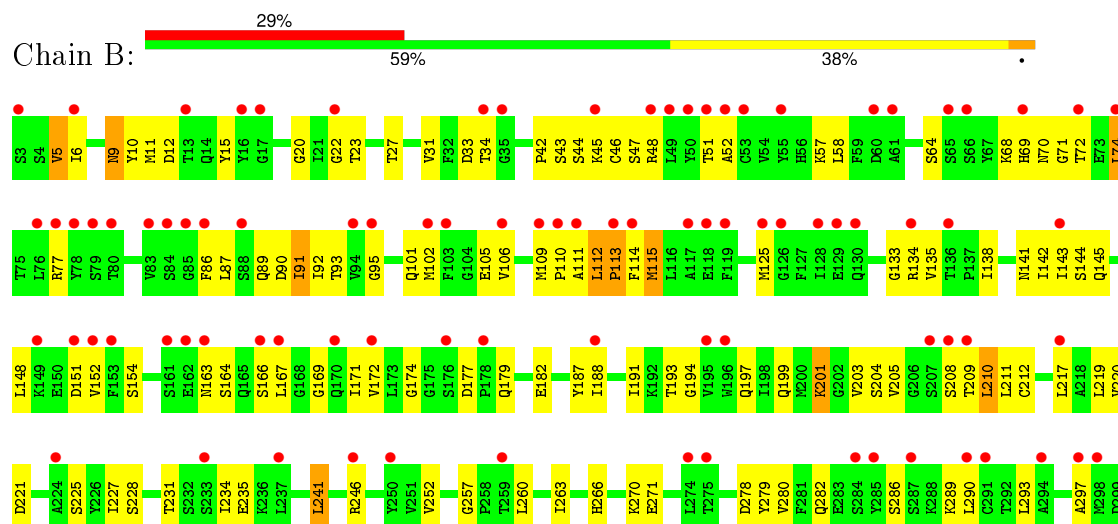
3 Residue-property plots

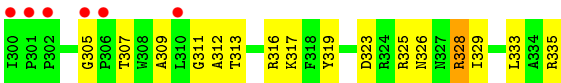
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Renin



• Molecule 1: Renin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	141.25Å 141.25Å 141.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 94.2 (49.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.251 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 25993 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	5498	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: 2IG, NAG

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	0.35	0/2632	0.66	0/3568
1	B	0.33	0/2632	0.65	0/3568
All	All	0.34	0/5264	0.66	0/7136

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	A	2572	0	2500	112	0
1	B	2572	0	2500	125	0
2	A	14	0	13	0	0
2	B	14	0	13	7	0
3	A	28	0	25	1	0
3	B	28	0	25	2	0
4	A	158	0	0	13	0
4	B	112	0	0	17	0
All	All	5498	0	5076	237	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 23.

All (237) 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:26:GLN:HE22	1:A:60:ASP:H	1.02	0.98
1:A:87:LEU:HB3	1:A:102:MET:HE1	1.48	0.96
1:B:326:ASN:HB2	1:B:328:ARG:HD2	1.53	0.91
1:A:235:GLU:HG3	4:A:1036:HOH:O	1.72	0.90
1:B:208:SER:HB2	4:B:990:HOH:O	1.73	0.87
1:A:276:SER:O	1:A:280:VAL:HG12	1.75	0.85
1:A:275:THR:HG21	4:A:993:HOH:O	1.77	0.83
1:B:252:VAL:HG23	4:B:996:HOH:O	1.80	0.81
1:B:191:ILE:HG13	4:B:1005:HOH:O	1.80	0.80
1:B:217:LEU:HD22	4:B:1005:HOH:O	1.80	0.80
1:A:152:VAL:HG12	1:A:323:ASP:HA	1.63	0.79
1:B:48:ARG:HH12	1:B:58:LEU:HD11	1.48	0.79
1:B:210:LEU:H	1:B:210:LEU:HD23	1.46	0.78
1:A:207:SER:HB2	4:A:1079:HOH:O	1.83	0.77
1:B:227:ILE:HG13	1:B:313:THR:HB	1.68	0.76
1:B:143:ILE:HG13	4:B:1087:HOH:O	1.86	0.75
1:A:275:THR:HG22	1:A:277:ALA:H	1.52	0.75
1:B:143:ILE:HD13	1:B:148:LEU:HD12	1.70	0.74
1:B:217:LEU:HB2	1:B:307:THR:HG22	1.71	0.73
1:B:286:SER:HB3	4:B:1066:HOH:O	1.87	0.72
1:B:71:GLY:H	2:B:986:NAG:H82	1.55	0.72
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.70	0.72
1:B:289:LYS:HB2	4:B:1066:HOH:O	1.90	0.72
1:B:323:ASP:HB3	1:B:328:ARG:HG2	1.73	0.71
1:B:152:VAL:HG12	1:B:323:ASP:HA	1.73	0.71
1:A:26:GLN:HE22	1:A:60:ASP:N	1.82	0.70
1:A:158:ASN:ND2	1:A:159:ARG:H	1.89	0.70
1:B:305:GLY:HA2	1:B:307:THR:HG23	1.75	0.68
1:B:191:ILE:HD11	1:B:199:GLN:HB2	1.77	0.67
1:B:5:VAL:HG13	1:B:171:ILE:HG23	1.75	0.67
1:B:70:ASN:HA	2:B:986:NAG:C8	2.24	0.66
1:A:208:SER:O	1:A:210:LEU:HD23	1.96	0.65
1:A:102:MET:HB2	4:A:1005:HOH:O	1.95	0.65
1:B:9:ASN:HD21	1:B:12:ASP:H	1.45	0.65
1:A:87:LEU:HB3	1:A:102:MET:CE	2.26	0.65
1:B:48:ARG:HH22	1:B:58:LEU:HD13	1.63	0.64
1:B:6:ILE:HG23	1:B:167:LEU:CD1	2.26	0.64
1:A:9:ASN:HD21	1:A:12:ASP:H	1.45	0.64
1:B:112:LEU:HD23	1:B:113:PRO:HA	1.80	0.63
1:A:226:TYR:HB3	1:A:294:ALA:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HG3	1:B:109:MET:HE1	1.79	0.62
1:B:9:ASN:C	1:B:9:ASN:HD22	2.02	0.62
1:A:130:GLN:HG3	4:A:1061:HOH:O	1.99	0.62
1:B:326:ASN:CB	1:B:328:ARG:HD2	2.28	0.62
1:B:197:GLN:OE1	1:B:307:THR:HG21	1.99	0.61
1:A:179:GLN:O	1:A:335:ARG:HD2	2.00	0.61
1:B:210:LEU:H	1:B:210:LEU:CD2	2.14	0.61
1:A:323:ASP:OD1	1:A:328:ARG:HD2	2.00	0.61
1:B:48:ARG:HH22	1:B:58:LEU:CD1	2.13	0.61
1:A:18:GLU:HG3	4:A:1131:HOH:O	1.99	0.61
1:A:9:ASN:HD22	1:A:9:ASN:C	2.04	0.61
1:B:220:VAL:HG21	1:B:329:ILE:HD13	1.83	0.60
1:A:163:ASN:HD22	1:A:163:ASN:H	1.49	0.60
1:A:300:ILE:O	1:A:305:GLY:HA3	2.01	0.60
1:A:161:SER:OG	1:A:163:ASN:ND2	2.36	0.59
1:B:5:VAL:HG13	1:B:171:ILE:CG2	2.32	0.59
1:B:225:SER:O	1:B:312:ALA:HB3	2.04	0.58
1:A:154:SER:HB3	1:A:319:TYR:CE1	2.38	0.58
1:A:253:LYS:HD2	1:A:256:GLU:OE2	2.03	0.58
1:B:203:VAL:HB	1:B:211:LEU:HB2	1.85	0.58
1:A:192:LYS:NZ	1:A:193:THR:O	2.36	0.57
1:B:323:ASP:OD1	1:B:328:ARG:HD3	2.04	0.57
1:B:142:ILE:O	1:B:145:GLN:HG2	2.04	0.57
1:A:45:LYS:HD2	4:A:1135:HOH:O	2.03	0.57
1:A:158:ASN:HD22	1:A:159:ARG:H	1.50	0.57
1:A:9:ASN:HD22	1:A:10:TYR:N	2.02	0.57
1:A:68:LYS:HB2	1:A:89:GLN:HB3	1.86	0.57
1:B:69:HIS:HA	4:B:1014:HOH:O	2.04	0.57
1:B:151:ASP:CB	4:B:995:HOH:O	2.53	0.57
1:A:266:HIS:HE1	1:A:269:GLY:HA2	1.71	0.56
1:B:52:ALA:HA	1:B:115:MET:HE2	1.88	0.56
1:B:182:GLU:HG2	1:B:335:ARG:HD3	1.88	0.56
1:B:231:THR:O	1:B:235:GLU:HG3	2.04	0.56
1:B:11:MET:O	1:B:12:ASP:HB2	2.06	0.56
1:A:325:ARG:HD2	4:A:1037:HOH:O	2.06	0.56
1:B:43:SER:O	1:B:58:LEU:HD22	2.04	0.55
1:B:111:ALA:O	1:B:115:MET:HB2	2.06	0.55
1:B:45:LYS:HD2	1:B:86:PHE:HZ	1.70	0.55
1:A:244:LYS:HB3	4:A:1108:HOH:O	2.07	0.55
1:B:106:VAL:HG11	1:B:109:MET:HE2	1.89	0.54
1:B:33:ASP:OD1	3:B:886:2IG:N2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HB2	1:B:307:THR:CG2	2.37	0.54
1:B:201:LYS:HE3	1:B:266:HIS:CD2	2.42	0.54
1:B:9:ASN:HD22	1:B:10:TYR:N	2.05	0.54
1:B:71:GLY:N	2:B:986:NAG:H82	2.23	0.54
1:A:163:ASN:ND2	1:A:163:ASN:O	2.41	0.53
1:B:266:HIS:HB2	4:B:988:HOH:O	2.08	0.53
1:B:9:ASN:C	1:B:9:ASN:ND2	2.62	0.53
1:B:15:TYR:O	1:B:31:VAL:HG22	2.08	0.53
1:B:151:ASP:HB2	4:B:995:HOH:O	2.07	0.53
1:B:33:ASP:HB2	3:B:886:2IG:H62	1.91	0.53
1:B:43:SER:HB2	1:B:105:GLU:HB3	1.90	0.53
1:A:197:GLN:CD	1:A:217:LEU:HD23	2.28	0.53
1:A:231:THR:O	1:A:235:GLU:HG2	2.09	0.52
1:B:167:LEU:HD11	1:B:169:GLY:O	2.10	0.52
1:A:247:LEU:HD22	1:A:248:PHE:CE2	2.45	0.52
1:B:228:SER:OG	1:B:309:ALA:HB3	2.09	0.52
1:B:148:LEU:HD22	1:B:174:GLY:HA3	1.91	0.51
1:A:227:ILE:HG13	1:A:313:THR:HB	1.92	0.51
1:B:70:ASN:HA	2:B:986:NAG:H81	1.92	0.51
1:B:280:VAL:HG22	1:B:293:LEU:HD22	1.92	0.51
1:A:87:LEU:HD13	1:A:102:MET:HE1	1.93	0.51
1:A:275:THR:CG2	1:A:276:SER:N	2.74	0.51
1:B:154:SER:HB3	1:B:319:TYR:CE1	2.46	0.51
1:B:289:LYS:HD2	4:B:1066:HOH:O	2.09	0.51
1:B:113:PRO:O	1:B:115:MET:N	2.44	0.51
1:A:188:ILE:CD1	1:A:267:LEU:HB3	2.41	0.51
1:A:212:CYS:SG	1:A:212:CYS:O	2.69	0.50
1:B:193:THR:HG22	1:B:194:GLY:N	2.26	0.50
1:B:71:GLY:H	2:B:986:NAG:C8	2.21	0.50
1:A:158:ASN:ND2	1:A:159:ARG:N	2.59	0.50
1:B:20:GLY:O	1:B:92:ILE:HA	2.12	0.50
1:B:187:TYR:HD2	1:B:328:ARG:HG3	1.77	0.50
1:A:159:ARG:HB3	4:A:1050:HOH:O	2.12	0.50
1:B:177:ASP:OD1	1:B:179:GLN:HB2	2.10	0.50
1:B:101:GLN:NE2	1:B:138:ILE:HA	2.27	0.50
1:B:141:ASN:O	1:B:144:SER:HB2	2.12	0.50
1:A:92:ILE:HD12	1:A:101:GLN:HB3	1.93	0.50
1:B:205:VAL:HB	1:B:210:LEU:HD21	1.94	0.50
1:A:9:ASN:ND2	1:A:9:ASN:C	2.65	0.49
1:A:74:LEU:HD13	1:A:87:LEU:HD21	1.95	0.49
1:B:187:TYR:CD2	1:B:328:ARG:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:C	1:A:237:LEU:HD23	2.32	0.49
1:A:188:ILE:HD13	1:A:267:LEU:HB3	1.95	0.49
1:B:112:LEU:HD23	1:B:113:PRO:CA	2.42	0.49
1:B:44:SER:C	1:B:46:CYS:H	2.15	0.49
1:A:33:ASP:OD1	3:A:885:2IG:N2	2.46	0.48
1:A:204:SER:OG	1:A:264:SER:HB2	2.14	0.48
1:B:27:THR:O	1:B:57:LYS:HD3	2.12	0.48
1:B:9:ASN:HD21	1:B:12:ASP:N	2.10	0.48
1:A:99:VAL:HG11	1:A:142:ILE:HG12	1.96	0.48
1:B:9:ASN:ND2	1:B:12:ASP:H	2.10	0.48
1:B:270:LYS:HG2	4:B:1095:HOH:O	2.14	0.48
1:A:275:THR:O	1:A:278:ASP:HB2	2.14	0.47
1:A:275:THR:HG22	1:A:276:SER:N	2.29	0.47
1:B:69:HIS:CG	1:B:70:ASN:N	2.81	0.47
1:B:280:VAL:HG22	1:B:293:LEU:CD2	2.45	0.47
1:B:209:THR:O	1:B:209:THR:HG22	2.14	0.47
1:B:5:VAL:HG23	4:B:1004:HOH:O	2.14	0.47
1:B:70:ASN:HA	2:B:986:NAG:H82	1.96	0.47
1:A:9:ASN:HD21	1:A:12:ASP:N	2.12	0.47
1:A:192:LYS:HD2	1:A:193:THR:H	1.80	0.47
1:A:22:GLY:HA2	1:A:90:ASP:OD2	2.14	0.47
1:B:133:GLY:C	1:B:134:ARG:HG3	2.35	0.46
1:A:247:LEU:HD22	1:A:248:PHE:CD2	2.50	0.46
1:A:127:PHE:CB	1:A:194:GLY:HA2	2.45	0.46
1:B:217:LEU:HD12	1:B:307:THR:HG22	1.98	0.46
1:B:51:THR:O	1:B:115:MET:HE3	2.15	0.46
1:B:143:ILE:CD1	1:B:148:LEU:HD12	2.42	0.46
1:A:203:VAL:HG23	1:A:212:CYS:HB3	1.96	0.46
1:A:26:GLN:NE2	1:A:59:PHE:HA	2.30	0.46
1:B:110:PRO:O	1:B:111:ALA:C	2.54	0.46
1:A:167:LEU:H	1:A:167:LEU:HD23	1.80	0.46
1:A:257:GLY:HA3	1:A:282:GLN:HE22	1.80	0.46
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.81	0.46
1:A:213:GLU:C	1:A:215:GLY:H	2.19	0.46
1:A:87:LEU:CB	1:A:102:MET:HE1	2.34	0.45
1:B:210:LEU:HD13	4:B:990:HOH:O	2.15	0.45
1:B:212:CYS:O	1:B:212:CYS:SG	2.74	0.45
1:B:45:LYS:HD2	1:B:86:PHE:CZ	2.49	0.45
1:B:278:ASP:OD1	1:B:317:LYS:HD3	2.16	0.45
1:B:113:PRO:C	1:B:115:MET:H	2.20	0.45
1:A:27:THR:O	1:A:57:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:HG2	4:B:1043:HOH:O	2.15	0.45
1:B:74:LEU:O	1:B:74:LEU:HD12	2.17	0.45
1:A:192:LYS:NZ	1:A:193:THR:CG2	2.80	0.45
1:A:97:ILE:HD13	1:A:142:ILE:HG23	1.99	0.45
1:B:188:ILE:HD12	1:B:188:ILE:N	2.32	0.45
1:A:225:SER:O	1:A:312:ALA:HB3	2.15	0.45
1:B:221:ASP:O	1:B:311:GLY:HA2	2.17	0.45
1:A:163:ASN:H	1:A:163:ASN:ND2	2.11	0.45
1:A:40:TRP:CD1	1:A:76:LEU:HD23	2.52	0.44
1:B:89:GLN:HB2	1:B:102:MET:SD	2.56	0.44
1:A:42:PRO:HB2	1:A:58:LEU:HD23	1.98	0.44
1:A:245:LYS:HD2	1:A:250:TYR:OH	2.18	0.44
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.33	0.44
1:A:9:ASN:ND2	1:A:12:ASP:H	2.13	0.44
1:B:52:ALA:HB3	1:B:109:MET:HB3	1.99	0.44
1:A:235:GLU:HB3	4:A:1143:HOH:O	2.17	0.44
1:B:312:ALA:O	1:B:316:ARG:HB2	2.17	0.44
1:A:192:LYS:HD2	1:A:193:THR:N	2.33	0.44
1:B:260:LEU:HB3	1:B:279:TYR:OH	2.18	0.44
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.33	0.44
1:A:163:ASN:ND2	1:A:163:ASN:N	2.66	0.44
1:B:134:ARG:CZ	2:B:986:NAG:H61	2.47	0.43
1:A:211:LEU:HD11	1:A:237:LEU:HB2	2.00	0.43
1:B:208:SER:O	1:B:210:LEU:HD22	2.19	0.43
1:B:22:GLY:HA2	1:B:90:ASP:OD1	2.18	0.43
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.77	0.43
1:A:231:THR:N	1:A:299:ASP:OD2	2.45	0.43
1:A:163:ASN:HD22	1:A:163:ASN:N	2.09	0.43
1:A:22:GLY:HA2	1:A:90:ASP:CG	2.39	0.43
1:B:91:ILE:O	1:B:91:ILE:HG13	2.18	0.43
1:A:69:HIS:CG	1:A:70:ASN:N	2.87	0.43
1:B:71:GLY:O	1:B:72:THR:C	2.58	0.43
1:B:70:ASN:O	1:B:87:LEU:O	2.36	0.43
1:A:112:LEU:HA	1:A:113:PRO:HA	1.81	0.43
1:B:87:LEU:HD11	1:B:135:VAL:HG21	2.01	0.43
1:A:97:ILE:HD13	1:A:142:ILE:CG2	2.49	0.42
1:A:251:VAL:HG21	1:A:290:LEU:HD13	2.01	0.42
1:B:151:ASP:HB3	1:B:325:ARG:HB2	1.99	0.42
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.81	0.42
1:A:266:HIS:CE1	1:A:269:GLY:HA2	2.52	0.42
1:B:234:ILE:HG13	1:B:297:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:THR:HG23	4:A:1112:HOH:O	2.18	0.42
1:A:87:LEU:HD13	1:A:102:MET:CE	2.50	0.42
1:B:172:VAL:HG23	4:B:1013:HOH:O	2.19	0.42
1:A:26:GLN:NE2	1:A:60:ASP:H	1.87	0.42
1:A:192:LYS:NZ	1:A:193:THR:HG22	2.34	0.42
1:A:246:ARG:HB3	1:A:247:LEU:H	1.75	0.42
1:A:101:GLN:HG3	1:A:102:MET:N	2.35	0.42
1:A:158:ASN:HD22	1:A:159:ARG:N	2.18	0.42
1:B:23:THR:O	1:B:64:SER:HA	2.19	0.42
1:B:220:VAL:CG2	1:B:329:ILE:HD13	2.49	0.41
1:A:48:ARG:HD3	1:A:48:ARG:HA	1.79	0.41
1:B:164:SER:OG	1:B:166:SER:HB2	2.20	0.41
1:A:326:ASN:HB2	1:A:328:ARG:CG	2.50	0.41
1:B:20:GLY:O	1:B:93:THR:N	2.44	0.41
1:A:90:ASP:OD2	1:A:91:ILE:N	2.50	0.41
1:A:19:ILE:HG13	1:A:19:ILE:O	2.21	0.41
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.90	0.41
1:A:325:ARG:C	1:A:326:ASN:HD22	2.25	0.41
1:B:204:SER:O	1:B:263:ILE:HA	2.21	0.41
1:A:159:ARG:CZ	4:A:1115:HOH:O	2.69	0.41
1:A:102:MET:HB3	1:A:102:MET:HE2	1.70	0.40
1:B:34:THR:HA	1:B:125:MET:HB2	2.03	0.40
1:B:257:GLY:HA3	1:B:282:GLN:HE22	1.85	0.40
1:A:313:THR:HA	1:A:316:ARG:NH2	2.35	0.40
1:A:76:LEU:HB2	1:A:83:VAL:HG23	2.02	0.40
1:B:9:ASN:HD21	1:B:12:ASP:HA	1.87	0.40
1:A:127:PHE:CG	1:A:194:GLY:HA2	2.57	0.40
1:A:178:PRO:HA	1:A:181:TYR:CE1	2.56	0.40
1:A:23:THR:O	1:A:64:SER:HA	2.22	0.40
1:A:276:SER:HA	1:A:279:TYR:CE2	2.57	0.40
1:B:48:ARG:NH1	1:B:58:LEU:HD11	2.27	0.40
1:A:91:ILE:HG13	1:A:91:ILE:O	2.21	0.40
1:A:47:SER:OG	1:A:49:LEU: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	331/333 (99%)	306 (92%)	23 (7%)	2 (1%)	30	59
1	B	331/333 (99%)	303 (92%)	24 (7%)	4 (1%)	16	39
All	All	662/666 (99%)	609 (92%)	47 (7%)	6 (1%)	21	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	B	114	PHE
1	A	270	LYS
1	B	246	ARG
1	B	47	SER
1	B	95	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	284/284 (100%)	270 (95%)	14 (5%)	31	61
1	B	284/284 (100%)	268 (94%)	16 (6%)	26	54
All	All	568/568 (100%)	538 (95%)	30 (5%)	28	57

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	49	LEU
1	A	76	LEU
1	A	93	THR
1	A	113	PRO
1	A	158	ASN
1	A	163	ASN
1	A	173	LEU
1	A	210	LEU
1	A	226	TYR
1	A	247	LEU
1	A	252	VAL
1	A	328	ARG
1	A	333	LEU
1	B	5	VAL
1	B	9	ASN
1	B	68	LYS
1	B	74	LEU
1	B	91	ILE
1	B	112	LEU
1	B	113	PRO
1	B	115	MET
1	B	163	ASN
1	B	201	LYS
1	B	210	LEU
1	B	219	LEU
1	B	241	LEU
1	B	290	LEU
1	B	328	ARG
1	B	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	101	GLN
1	A	141	ASN
1	A	145	GLN
1	A	158	ASN
1	A	163	ASN
1	A	189	ASN
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	266	HIS
1	A	282	GLN
1	A	296	HIS
1	A	326	ASN
1	B	9	ASN
1	B	26	GLN
1	B	56	HIS
1	B	101	GLN
1	B	141	ASN
1	B	145	GLN
1	B	186	HIS
1	B	189	ASN
1	B	266	HIS
1	B	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
3	2IG	A	885	-	29,31,31	1.36	4 (13%)	32,44,44	1.35	4 (12%)
2	NAG	A	985	1	14,14,15	0.50	0	15,19,21	0.88	1 (6%)
3	2IG	B	886	-	29,31,31	1.37	5 (17%)	32,44,44	1.34	4 (12%)
2	NAG	B	986	1	14,14,15	0.71	1 (7%)	15,19,21	0.72	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	2IG	A	885	-	-	0/11/11/11	0/4/4/4
2	NAG	A	985	1	-	0/6/23/26	0/1/1/1
3	2IG	B	886	-	-	0/11/11/11	0/4/4/4
2	NAG	B	986	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	886	2IG	C22-C21	2.06	1.43	1.38
2	B	986	NAG	C1-C2	2.15	1.55	1.52
3	B	886	2IG	C7-C12	2.18	1.44	1.39
3	A	885	2IG	C22-C21	2.19	1.43	1.38
3	B	886	2IG	C22-C17	2.59	1.42	1.36
3	A	885	2IG	C22-C17	2.90	1.43	1.36
3	A	885	2IG	C21-C20	3.01	1.43	1.36
3	B	886	2IG	C21-C20	3.09	1.43	1.36
3	B	886	2IG	C8-C7	4.10	1.45	1.36
3	A	885	2IG	C8-C7	4.13	1.45	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	886	2IG	C4-C3-N2	-3.32	119.66	123.87
3	A	885	2IG	C4-C3-N2	-3.26	119.74	123.87
3	A	885	2IG	C11-C12-C4	-2.76	113.25	122.16
3	B	886	2IG	C11-C12-C4	-2.54	113.97	122.16
2	A	985	NAG	C2-N2-C7	-2.45	119.89	123.04
3	B	886	2IG	C4-C1-N1	2.17	123.88	122.55
3	A	885	2IG	C4-C1-N1	2.18	123.89	122.55
3	B	886	2IG	C7-C12-C4	4.11	127.66	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	885	2IG	C7-C12-C4	4.45	128.22	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	885	2IG	1	0
3	B	886	2IG	2	0
2	B	986	NAG	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/333 (100%)	1.79	121 (36%) 0 0	18, 34, 55, 80	0
1	B	333/333 (100%)	1.58	96 (28%) 1 0	21, 42, 71, 92	0
All	All	666/666 (100%)	1.68	217 (32%) 1 0	18, 37, 66, 92	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	SER	5.2
1	B	134	ARG	5.0
1	A	188	ILE	5.0
1	A	99	VAL	4.8
1	A	247	LEU	4.6
1	B	53	CYS	4.5
1	A	191	ILE	4.4
1	B	52	ALA	4.3
1	B	55	TYR	4.3
1	A	180	HIS	4.2
1	A	200	MET	4.2
1	B	209	THR	4.1
1	A	19	ILE	4.0
1	A	193	THR	4.0
1	A	205	VAL	4.0
1	A	97	ILE	4.0
1	B	208	SER	3.9
1	B	77	ARG	3.9
1	A	209	THR	3.8
1	B	48	ARG	3.8
1	B	49	LEU	3.8
1	A	157	TYR	3.8
1	A	93	THR	3.8
1	B	51	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	331	PHE	3.6
1	B	294	ALA	3.6
1	A	329	ILE	3.6
1	A	306	PRO	3.5
1	B	78	TYR	3.5
1	A	248	PHE	3.5
1	A	38	ASN	3.5
1	B	95	GLY	3.5
1	A	334	ALA	3.5
1	B	162	GLU	3.5
1	B	114	PHE	3.4
1	A	186	HIS	3.4
1	A	175	GLY	3.4
1	B	306	PRO	3.4
1	A	30	VAL	3.4
1	B	80	THR	3.4
1	B	61	ALA	3.4
1	B	161	SER	3.4
1	A	82	THR	3.4
1	A	31	VAL	3.3
1	A	111	ALA	3.3
1	A	187	TYR	3.2
1	B	66	SER	3.2
1	A	71	GLY	3.2
1	B	84	SER	3.2
1	B	300	ILE	3.2
1	A	211	LEU	3.2
1	B	3	SER	3.2
1	B	274	LEU	3.1
1	A	151	ASP	3.1
1	A	78	TYR	3.1
1	A	269	GLY	3.1
1	A	153	PHE	3.1
1	A	330	GLY	3.1
1	B	83	VAL	3.0
1	A	171	ILE	3.0
1	A	94	VAL	3.0
1	A	92	ILE	3.0
1	A	182	GLU	3.0
1	B	172	VAL	3.0
1	A	290	LEU	2.9
1	B	275	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	2.9
1	A	137	PRO	2.9
1	A	173	LEU	2.9
1	B	310	LEU	2.9
1	B	178	PRO	2.9
1	A	190	LEU	2.8
1	B	152	VAL	2.8
1	A	320	THR	2.8
1	A	75	THR	2.8
1	B	119	PHE	2.8
1	A	319	TYR	2.8
1	A	91	ILE	2.8
1	A	125	MET	2.8
1	B	207	SER	2.8
1	A	194	GLY	2.8
1	B	50	TYR	2.8
1	B	69	HIS	2.8
1	A	135	VAL	2.8
1	B	291	CYS	2.8
1	A	8	THR	2.8
1	B	128	ILE	2.7
1	A	195	VAL	2.7
1	A	40	TRP	2.7
1	A	221	ASP	2.7
1	A	60	ASP	2.7
1	A	177	ASP	2.7
1	B	117	ALA	2.7
1	A	67	TYR	2.6
1	A	225	SER	2.6
1	B	102	MET	2.6
1	B	233	SER	2.6
1	B	151	ASP	2.6
1	A	315	ILE	2.6
1	A	24	PRO	2.6
1	B	16	TYR	2.6
1	A	231	THR	2.6
1	A	288	LYS	2.6
1	B	176	SER	2.6
1	A	312	ALA	2.6
1	A	27	THR	2.6
1	B	237	LEU	2.6
1	B	284	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	111	ALA	2.6
1	B	72	THR	2.6
1	B	285	TYR	2.6
1	B	86	PHE	2.6
1	A	148	LEU	2.5
1	B	297	ALA	2.5
1	B	110	PRO	2.5
1	B	143	ILE	2.5
1	B	287	SER	2.5
1	A	179	GLN	2.5
1	A	80	THR	2.5
1	A	150	GLU	2.5
1	B	13	THR	2.5
1	B	136	THR	2.5
1	A	155	PHE	2.5
1	A	327	ASN	2.5
1	A	138	ILE	2.5
1	A	198	ILE	2.5
1	A	291	CYS	2.5
1	A	295	ILE	2.5
1	A	276	SER	2.5
1	B	126	GLY	2.5
1	A	219	LEU	2.4
1	A	161	SER	2.4
1	A	156	TYR	2.4
1	B	60	ASP	2.4
1	A	104	GLY	2.4
1	B	74	LEU	2.4
1	B	34	THR	2.4
1	A	266	HIS	2.4
1	A	304	THR	2.4
1	A	318	PHE	2.4
1	B	217	LEU	2.4
1	A	216	CYS	2.4
1	B	246	ARG	2.4
1	B	45	LYS	2.4
1	A	281	PHE	2.4
1	A	298	MET	2.4
1	A	168	GLY	2.4
1	A	28	PHE	2.3
1	A	267	LEU	2.3
1	B	85	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	94	VAL	2.3
1	A	201	LYS	2.3
1	B	103	PHE	2.3
1	B	195	VAL	2.3
1	A	158	ASN	2.3
1	B	259	THR	2.3
1	B	17	GLY	2.3
1	A	152	VAL	2.3
1	A	308	TRP	2.3
1	B	129	GLU	2.3
1	B	6	ILE	2.3
1	A	192	LYS	2.3
1	A	287	SER	2.3
1	B	167	LEU	2.3
1	A	54	VAL	2.3
1	A	101	GLN	2.3
1	A	166	SER	2.2
1	A	50	TYR	2.2
1	A	273	THR	2.2
1	A	328	ARG	2.2
1	A	196	TRP	2.2
1	A	185	PHE	2.2
1	B	109	MET	2.2
1	A	203	VAL	2.2
1	B	88	SER	2.2
1	B	298	MET	2.2
1	B	188	ILE	2.2
1	B	118	GLU	2.2
1	A	307	THR	2.2
1	A	16	TYR	2.2
1	B	130	GLN	2.2
1	A	81	GLY	2.2
1	B	224	ALA	2.2
1	A	227	ILE	2.2
1	A	264	SER	2.2
1	A	172	VAL	2.2
1	A	95	GLY	2.1
1	A	202	GLY	2.1
1	B	153	PHE	2.1
1	B	163	ASN	2.1
1	A	77	ARG	2.1
1	B	290	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	2.1
1	B	302	PRO	2.1
1	A	159	ARG	2.1
1	B	170	GLN	2.1
1	B	35	GLY	2.1
1	B	65	SER	2.1
1	B	305	GLY	2.1
1	B	113	PRO	2.1
1	B	250	TYR	2.1
1	A	98	THR	2.1
1	B	149	LYS	2.1
1	A	251	VAL	2.1
1	A	139	PHE	2.1
1	A	316	ARG	2.1
1	B	22	GLY	2.1
1	A	224	ALA	2.1
1	A	297	ALA	2.1
1	B	125	MET	2.0
1	A	121	GLY	2.0
1	B	106	VAL	2.0
1	B	196	TRP	2.0
1	B	166	SER	2.0
1	A	21	ILE	2.0
1	A	305	GLY	2.0
1	B	76	LEU	2.0

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	2IG	A	885	28/28	0.81	0.33	0.60	24,25,30,31	0
3	2IG	B	886	28/28	0.79	0.32	0.22	34,45,47,48	0
2	NAG	B	986	14/15	0.55	0.37	0.21	78,80,81,81	0
2	NAG	A	985	14/15	0.72	0.28	-	44,48,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.