Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:12 AM GMT

PDB ID	:	2G27
Title	:	Ketopiperazine-Based Renin Inhibitors: Optimization of the "C" Ring
Authors	:	Holsworth, D.D.; Jalaiea, M.; Zhanga, E.; Mcconnella, P.
Deposited on	:	2006-02-15
Resolution	:	2.90 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:

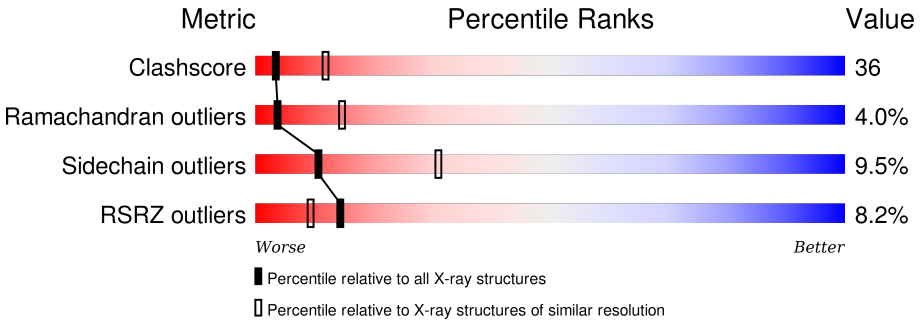
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	333	11% 46% 43% 10%
1	B	333	5% 51% 38% 9%

2 Entry composition

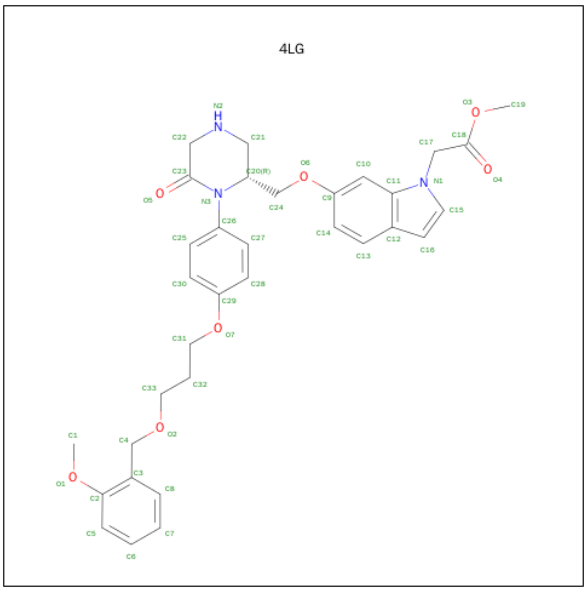
There are 2 unique types of molecules in this entry. The entry contains 5154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	328	Total	C	N	O	S	0	0	0
			2534	1622	409	489	14			
1	B	328	Total	C	N	O	S	0	0	0
			2534	1622	409	489	14			

- Molecule 2 is METHYL (6-{[(2R)-1-(4-{3-[(2-METHOXYBENZYL)OXY]PROPOXY}PHENYL)-6-OXOPIPERAZIN-2-YL]METHOXY}-1H-INDOL-1-YL)ACETATE (three-letter code: 4LG) (formula: $C_{33}H_{37}N_3O_7$).



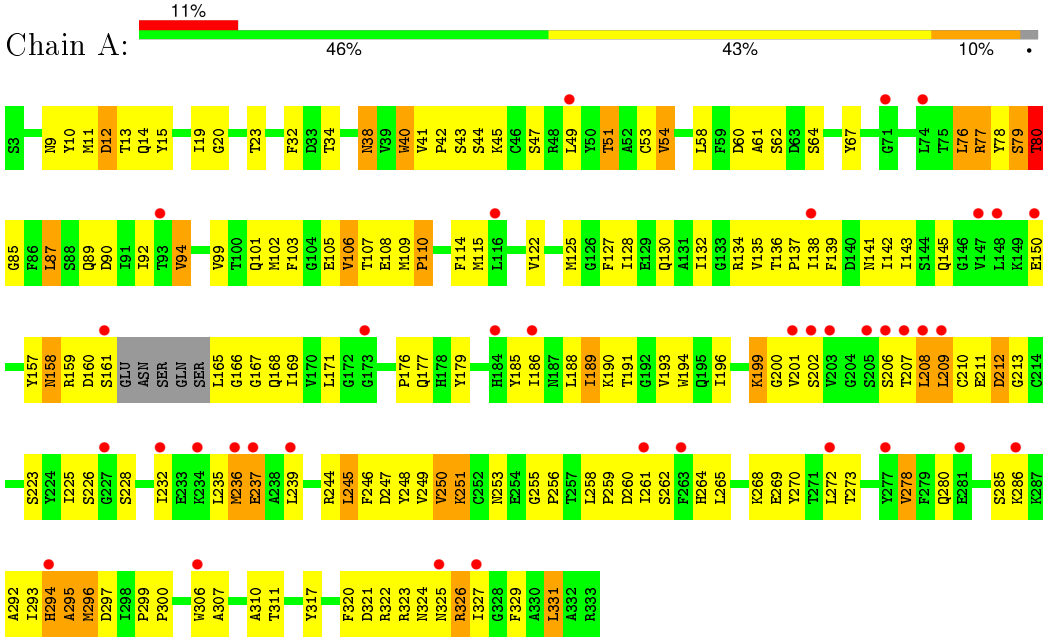
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			43	33	3	7		
2	A	1	Total	C	N	O	0	0
			43	33	3	7		

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.

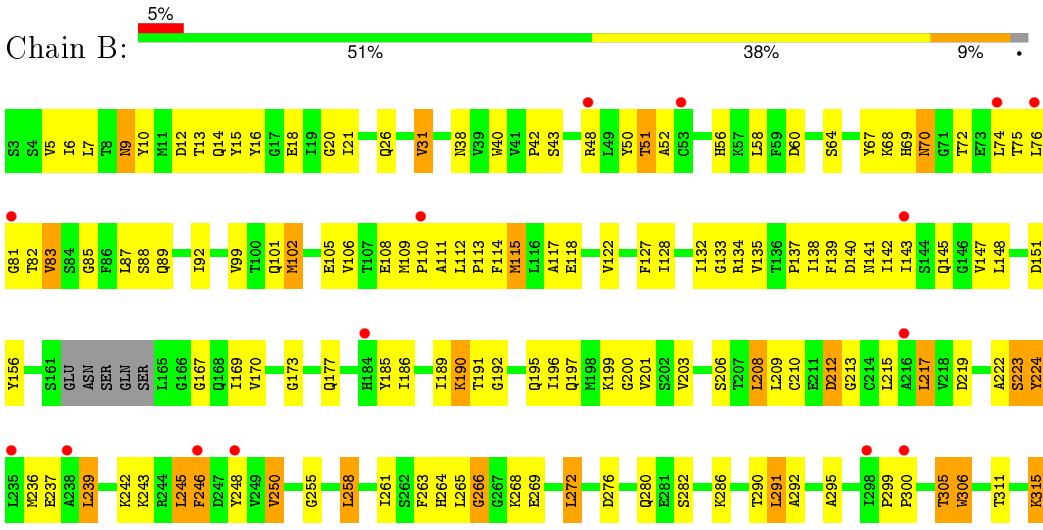
- Molecule 1: Renin

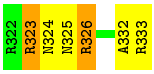
Chain A:



- Molecule 1: Renin

Chain B:




R322
R323
N324
N325
R326
A332
R333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	141.41Å 141.41Å 141.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 47.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 91.1 (47.14-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.310 0.281 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.6	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 20900 reflections	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: 4LG

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	0.39	0/2593	0.72	1/3514 (0.0%)
1	B	0.44	0/2593	0.75	1/3514 (0.0%)
All	All	0.42	0/5186	0.73	2/7028 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	306	TRP	N-CA-C	-6.36	93.82	111.00
1	A	80	THR	N-CA-C	-5.96	94.91	111.00

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	2534	0	2470	190	0
1	B	2534	0	2470	178	0
2	A	43	0	37	9	0
2	B	43	0	37	12	0
All	All	5154	0	5014	371	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 36.

All (371) 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:82:THR:HG23	1:A:83:VAL:H	1.02	1.10
1:B:152:VAL:HG12	1:B:321:ASP:HA	1.30	1.09
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.35	1.06
1:A:158:ASN:ND2	1:A:159:ARG:H	1.53	1.05
1:A:158:ASN:HD22	1:A:159:ARG:N	1.56	1.04
1:A:77:ARG:H	1:A:77:ARG:HD2	1.20	1.04
1:B:323:ARG:HH11	1:B:323:ARG:HG3	1.34	0.93
1:A:82:THR:HG23	1:A:83:VAL:N	1.84	0.93
1:B:324:ASN:HB2	1:B:326:ARG:HD2	1.54	0.90
1:A:82:THR:CG2	1:A:83:VAL:H	1.86	0.89
1:B:43:SER:HB2	1:B:105:GLU:HB3	1.54	0.88
1:A:128:ILE:HD13	1:A:137:PRO:HD3	1.56	0.87
1:B:245:LEU:HD23	1:B:246:PHE:N	1.90	0.87
1:B:14:GLN:HA	2:B:803:4LG:O4	1.74	0.87
1:A:152:VAL:HG12	1:A:321:ASP:HA	1.58	0.85
1:B:315:LYS:HG2	1:B:316:PHE:CE1	2.13	0.83
1:A:130:GLN:NE2	1:A:193:VAL:HG22	1.93	0.83
1:B:76:LEU:HD11	1:B:132:ILE:HG13	1.61	0.82
1:B:14:GLN:HG2	2:B:803:4LG:H15	1.61	0.81
1:A:78:TYR:H	1:A:81:GLY:HA2	1.45	0.81
1:B:217:LEU:HD22	1:B:219:ASP:HB2	1.63	0.80
1:A:51:THR:HB	1:A:115:MET:HG3	1.63	0.80
1:A:158:ASN:HD22	1:A:159:ARG:H	0.83	0.80
1:A:19:ILE:HG22	1:A:94:VAL:HG13	1.62	0.80
1:B:245:LEU:HD23	1:B:246:PHE:H	1.46	0.79
1:A:77:ARG:N	1:A:77:ARG:HD2	1.97	0.79
1:A:82:THR:HG23	1:A:110:PRO:HD3	1.66	0.78
1:A:249:VAL:HG21	1:A:288:LEU:HD13	1.66	0.78
1:B:101:GLN:HA	1:B:101:GLN:HE21	1.51	0.76
1:B:72:THR:HB	1:B:87:LEU:HD12	1.67	0.75
1:B:203:VAL:HB	1:B:208:LEU:HD11	1.67	0.75
1:A:158:ASN:ND2	1:A:159:ARG:N	2.24	0.75
1:B:258:LEU:N	1:B:258:LEU:HD23	2.01	0.74
1:B:128:ILE:HG13	1:B:137:PRO:HD3	1.68	0.73
1:A:130:GLN:HE22	1:A:193:VAL:HG22	1.53	0.73
1:A:11:MET:O	1:A:13:THR:HG23	1.87	0.73
1:A:132:ILE:O	1:A:135:VAL:HG23	1.90	0.72
1:B:87:LEU:HD21	1:B:135:VAL:HG21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:HD21	1:B:12:ASP:H	1.38	0.71
1:A:268:LYS:NZ	1:A:269:GLU:H	1.89	0.71
1:A:9:ASN:OD1	1:A:160:ASP:HB2	1.90	0.70
1:A:40:TRP:HB3	2:A:804:4LG:H331	1.73	0.70
1:A:211:GLU:O	1:A:212:ASP:HB2	1.92	0.70
1:A:87:LEU:HD13	1:A:102:MET:HE2	1.73	0.70
1:A:235:LEU:O	1:A:239:LEU:HG	1.92	0.69
1:B:321:ASP:HB3	1:B:326:ARG:HG2	1.75	0.69
1:B:79:SER:O	1:B:80:THR:HG22	1.93	0.69
1:B:268:LYS:HG3	1:B:269:GLU:N	2.07	0.69
1:A:47:SER:OG	1:A:49:LEU:HD23	1.94	0.68
1:A:208:LEU:O	1:A:209:LEU:HG	1.94	0.68
1:A:45:LYS:O	1:A:45:LYS:HD3	1.94	0.67
1:A:150:GLU:HB2	1:A:152:VAL:HG22	1.74	0.67
1:A:87:LEU:HD13	1:A:102:MET:CE	2.25	0.67
1:B:51:THR:HB	1:B:115:MET:SD	2.35	0.67
1:B:170:VAL:HB	1:B:173:GLY:O	1.95	0.67
1:A:199:LYS:HB3	1:A:264:HIS:HD2	1.58	0.66
1:B:139:PHE:O	1:B:143:ILE:HG12	1.95	0.66
1:A:76:LEU:HD13	1:A:76:LEU:O	1.96	0.66
1:B:82:THR:HG23	1:B:110:PRO:HG3	1.77	0.66
1:B:89:GLN:HB2	1:B:102:MET:HE1	1.78	0.66
1:B:201:VAL:HG23	1:B:209:LEU:HB2	1.78	0.66
1:A:76:LEU:HB3	1:A:132:ILE:HD11	1.77	0.65
1:B:245:LEU:HD23	1:B:246:PHE:CB	2.26	0.65
1:A:249:VAL:HG12	1:A:290:THR:HA	1.78	0.65
1:B:50:TYR:CZ	1:B:108:GLU:HB2	2.32	0.65
1:B:208:LEU:HD13	1:B:208:LEU:H	1.61	0.65
1:B:127:PHE:CB	1:B:192:GLY:HA2	2.28	0.64
1:B:224:TYR:HB3	1:B:292:ALA:O	1.97	0.64
1:B:74:LEU:HD21	1:B:87:LEU:HG	1.78	0.64
1:B:154:SER:HB3	1:B:317:TYR:CE1	2.33	0.64
1:A:82:THR:CG2	1:A:110:PRO:HD3	2.28	0.64
1:B:83:VAL:HA	1:B:108:GLU:O	1.98	0.64
1:A:101:GLN:HG3	1:A:102:MET:N	2.14	0.63
1:A:13:THR:O	2:A:804:4LG:O4	2.16	0.63
1:A:43:SER:O	1:A:58:LEU:HD13	1.96	0.63
1:A:87:LEU:HD23	1:A:103:PHE:O	1.99	0.63
1:B:76:LEU:CD1	1:B:132:ILE:HG13	2.27	0.63
1:A:78:TYR:O	1:A:81:GLY:N	2.32	0.63
1:B:323:ARG:NH1	1:B:323:ARG:HG3	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:MET:HB3	1:B:135:VAL:CG1	2.29	0.62
1:A:199:LYS:HB3	1:A:264:HIS:CD2	2.35	0.62
1:A:268:LYS:HZ2	1:A:269:GLU:H	1.46	0.62
1:A:128:ILE:CD1	1:A:137:PRO:HD3	2.29	0.62
1:B:127:PHE:HB2	1:B:192:GLY:HA2	1.82	0.62
1:A:185:TYR:C	1:A:186:ILE:HD12	2.20	0.62
1:B:26:GLN:HE22	1:B:60:ASP:H	1.47	0.62
1:A:223:SER:O	1:A:310:ALA:HB3	2.00	0.61
1:B:111:ALA:O	1:B:115:MET:HB2	2.00	0.61
1:A:106:VAL:HG11	1:A:109:MET:HG3	1.81	0.61
1:A:41:VAL:O	1:A:106:VAL:HG23	2.00	0.61
1:B:199:LYS:NZ	1:B:266:GLY:HA2	2.15	0.61
1:A:43:SER:HB2	1:A:105:GLU:CB	2.23	0.61
1:B:315:LYS:HG2	1:B:316:PHE:CD1	2.34	0.61
1:A:38:ASN:HD21	1:A:132:ILE:H	1.48	0.61
1:A:99:VAL:HG11	1:A:142:ILE:HG12	1.81	0.61
1:B:152:VAL:CG1	1:B:321:ASP:HA	2.19	0.61
1:A:20:GLY:O	1:A:92:ILE:HA	2.01	0.61
1:B:236:MET:HG3	1:B:248:TYR:CD2	2.36	0.61
1:B:210:CYS:SG	1:B:210:CYS:O	2.58	0.60
1:A:253:ASN:CG	1:A:285:SER:HA	2.22	0.60
1:B:89:GLN:HB2	1:B:102:MET:CE	2.31	0.60
1:B:99:VAL:HG21	1:B:141:ASN:HB3	1.84	0.60
1:A:14:GLN:HA	2:A:804:4LG:O4	2.01	0.60
1:A:14:GLN:HG2	2:A:804:4LG:H15	1.84	0.60
1:B:9:ASN:HD21	1:B:12:ASP:N	2.00	0.60
1:A:245:LEU:HD22	1:A:246:PHE:CE1	2.37	0.59
1:A:154:SER:HB3	1:A:317:TYR:CE1	2.37	0.59
1:A:77:ARG:CD	1:A:77:ARG:H	2.02	0.59
1:B:189:ILE:HD11	1:B:197:GLN:HB2	1.85	0.59
1:A:211:GLU:O	1:A:212:ASP:CB	2.50	0.58
1:A:196:ILE:CD1	1:A:265:LEU:HD22	2.33	0.58
1:A:209:LEU:HD11	1:A:235:LEU:HB2	1.83	0.58
1:B:199:LYS:O	1:B:264:HIS:HB3	2.04	0.58
1:A:76:LEU:O	1:A:83:VAL:HG13	2.03	0.58
1:B:215:LEU:CB	1:B:305:THR:HG22	2.34	0.58
1:A:206:SER:HB2	1:A:208:LEU:HG	1.86	0.58
1:A:138:ILE:O	1:A:142:ILE:HG13	2.04	0.58
1:A:82:THR:O	1:A:83:VAL:O	2.23	0.57
1:A:253:ASN:OD1	1:A:285:SER:HA	2.04	0.57
1:A:226:SER:HB2	1:A:296:MET:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:HG3	1:B:191:THR:N	2.20	0.57
1:A:81:GLY:O	1:A:82:THR:HG22	2.04	0.57
1:B:239:LEU:HD21	1:B:261:ILE:HD11	1.85	0.57
1:A:150:GLU:CB	1:A:152:VAL:HG22	2.35	0.56
1:A:76:LEU:HD13	1:A:83:VAL:HG13	1.87	0.56
1:A:122:VAL:HG23	2:A:804:4LG:H11	1.87	0.56
1:B:323:ARG:CG	1:B:323:ARG:HH11	2.11	0.56
1:B:78:TYR:O	1:B:79:SER:C	2.44	0.56
1:B:143:ILE:CD1	1:B:148:LEU:HD12	2.35	0.56
1:A:134:ARG:HH21	1:A:134:ARG:HB2	1.70	0.56
1:B:106:VAL:HG21	2:B:803:4LG:H331	1.86	0.56
1:A:89:GLN:O	1:A:90:ASP:HB2	2.04	0.56
1:B:38:ASN:HB2	1:B:40:TRP:CZ3	2.41	0.55
1:B:191:THR:HG22	1:B:192:GLY:N	2.22	0.55
1:B:10:TYR:HB3	1:B:14:GLN:HB2	1.89	0.55
1:B:13:THR:O	2:B:803:4LG:O4	2.25	0.55
1:A:210:CYS:SG	1:A:210:CYS:O	2.65	0.55
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.22	0.54
1:B:154:SER:HB3	1:B:317:TYR:HE1	1.73	0.54
1:A:165:LEU:HD11	1:A:167:GLY:O	2.07	0.54
1:B:272:LEU:HD23	1:B:276:ASP:HB3	1.90	0.54
1:A:78:TYR:H	1:A:81:GLY:CA	2.18	0.54
1:B:250:VAL:HG21	1:B:258:LEU:HD11	1.88	0.54
1:A:186:ILE:N	1:A:186:ILE:HD12	2.22	0.54
1:B:232:ILE:HB	1:B:295:ALA:HB2	1.90	0.54
1:B:177:GLN:HA	1:B:333:ARG:HH21	1.73	0.54
1:B:101:GLN:HA	1:B:101:GLN:NE2	2.21	0.54
1:B:74:LEU:N	1:B:85:GLY:O	2.39	0.53
1:B:195:GLN:OE1	1:B:215:LEU:HD22	2.08	0.53
1:A:152:VAL:HG12	1:A:321:ASP:CA	2.35	0.53
1:A:76:LEU:HB3	1:A:132:ILE:CD1	2.38	0.53
1:B:245:LEU:HD23	1:B:246:PHE:CA	2.38	0.53
1:A:235:LEU:C	1:A:235:LEU:HD23	2.29	0.53
1:A:106:VAL:CG1	1:A:109:MET:HG3	2.39	0.53
1:B:324:ASN:CB	1:B:326:ARG:HD2	2.33	0.53
1:B:5:VAL:CG1	1:B:169:ILE:HB	2.39	0.53
1:B:245:LEU:CD2	1:B:246:PHE:N	2.67	0.53
1:B:79:SER:O	1:B:80:THR:CB	2.57	0.53
1:B:79:SER:O	1:B:80:THR:CG2	2.57	0.53
1:A:83:VAL:HA	1:A:108:GLU:O	2.09	0.53
1:A:165:LEU:HD12	1:A:166:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HA	1:A:179:TYR:CE1	2.44	0.52
1:A:190:LYS:HG3	1:A:190:LYS:O	2.08	0.52
1:A:159:ARG:O	1:A:160:ASP:HB3	2.09	0.52
1:B:190:LYS:HG3	1:B:191:THR:O	2.10	0.52
1:A:201:VAL:H	1:A:210:CYS:HB3	1.74	0.52
1:A:165:LEU:HD12	1:A:166:GLY:H	1.73	0.52
1:B:48:ARG:NH1	1:B:58:LEU:HD13	2.25	0.52
1:B:75:THR:O	1:B:76:LEU:HD13	2.09	0.52
1:A:78:TYR:O	1:A:80:THR:HG22	2.09	0.51
1:B:102:MET:HB3	1:B:135:VAL:HG13	1.91	0.51
1:B:7:LEU:HB2	1:B:167:GLY:C	2.30	0.51
1:A:78:TYR:O	1:A:80:THR:N	2.44	0.51
1:B:232:ILE:HG21	1:B:295:ALA:HB2	1.93	0.51
1:B:291:LEU:N	1:B:291:LEU:HD23	2.25	0.51
1:A:82:THR:CG2	1:A:83:VAL:N	2.56	0.51
1:A:101:GLN:HE22	1:A:138:ILE:HA	1.75	0.51
1:A:291:LEU:C	1:A:293:ILE:H	2.14	0.51
1:B:224:TYR:HA	1:B:311:THR:OG1	2.11	0.51
1:B:9:ASN:ND2	1:B:12:ASP:H	2.04	0.51
1:B:208:LEU:CD1	1:B:208:LEU:H	2.24	0.51
1:A:136:THR:HG21	1:A:141:ASN:ND2	2.26	0.50
1:A:260:ASP:C	1:A:261:ILE:HD13	2.32	0.50
1:A:10:TYR:HB3	1:A:14:GLN:HB2	1.93	0.50
1:B:42:PRO:HB2	1:B:58:LEU:HD23	1.92	0.50
1:B:10:TYR:CD2	1:B:118:GLU:HG3	2.46	0.50
1:A:9:ASN:HD22	1:A:10:TYR:N	2.10	0.50
1:A:278:VAL:HG12	1:A:291:LEU:HD22	1.94	0.50
1:B:20:GLY:O	1:B:92:ILE:HA	2.12	0.50
1:A:82:THR:HG22	1:A:110:PRO:HB3	1.94	0.50
1:B:14:GLN:CG	2:B:803:4LG:H15	2.38	0.50
1:A:232:ILE:HG13	1:A:295:ALA:HA	1.93	0.50
1:B:88:SER:O	1:B:102:MET:HE2	2.12	0.49
1:A:83:VAL:HB	1:A:110:PRO:HD2	1.93	0.49
1:B:203:VAL:HB	1:B:208:LEU:CD1	2.39	0.49
1:A:188:LEU:HG	1:A:325:ASN:O	2.12	0.49
1:B:208:LEU:CD2	1:B:209:LEU:HG	2.42	0.49
1:B:245:LEU:CD2	1:B:246:PHE:H	2.20	0.49
1:B:48:ARG:HH12	1:B:58:LEU:HD13	1.77	0.49
1:A:151:ASP:OD2	1:A:322:ARG:HB2	2.13	0.49
1:A:9:ASN:HD21	1:A:12:ASP:N	2.11	0.49
1:B:21:ILE:HG12	1:B:92:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD22	1:A:259:PRO:HG2	1.94	0.49
1:B:75:THR:C	1:B:76:LEU:HD22	2.33	0.49
1:B:232:ILE:CB	1:B:295:ALA:HB2	2.42	0.49
2:B:803:4LG:H42	2:B:803:4LG:H13A	1.94	0.48
1:B:201:VAL:CG2	1:B:209:LEU:HB2	2.43	0.48
1:A:128:ILE:HD13	1:A:136:THR:HA	1.96	0.48
1:A:262:SER:HA	1:A:270:TYR:O	2.14	0.48
1:A:237:GLU:C	1:A:239:LEU:H	2.16	0.48
1:A:42:PRO:HA	1:A:106:VAL:HG23	1.96	0.48
1:B:56:HIS:CE1	2:B:803:4LG:H6	2.48	0.48
1:B:76:LEU:HD22	1:B:76:LEU:N	2.28	0.48
1:B:78:TYR:H	1:B:81:GLY:HA3	1.79	0.48
1:B:101:GLN:HE21	1:B:101:GLN:CA	2.16	0.48
1:A:15:TYR:CZ	1:A:157:TYR:HB3	2.48	0.48
1:A:202:SER:HB2	1:A:207:THR:HG23	1.95	0.48
1:A:78:TYR:O	1:A:79:SER:C	2.52	0.48
1:A:81:GLY:O	1:A:82:THR:CB	2.62	0.48
1:B:83:VAL:H	1:B:110:PRO:HD3	1.76	0.48
1:B:89:GLN:HE21	1:B:102:MET:CE	2.26	0.48
1:A:251:LYS:HD2	1:A:286:LYS:O	2.14	0.47
1:B:232:ILE:CG2	1:B:295:ALA:HB2	2.44	0.47
1:A:244:ARG:HB2	1:A:247:ASP:O	2.15	0.47
1:A:196:ILE:HD11	1:A:265:LEU:HD22	1.96	0.47
1:A:225:ILE:HG13	1:A:311:THR:HB	1.97	0.47
1:A:299:PRO:HA	1:A:300:PRO:HD3	1.71	0.47
1:B:263:PHE:N	1:B:263:PHE:CD1	2.82	0.47
1:A:23:THR:O	1:A:64:SER:HA	2.14	0.47
1:A:60:ASP:OD1	1:A:62:SER:HB2	2.14	0.47
1:B:40:TRP:CZ2	1:B:76:LEU:HD21	2.49	0.47
1:B:82:THR:OG1	1:B:83:VAL:N	2.48	0.47
1:B:323:ARG:NH1	1:B:323:ARG:CG	2.70	0.47
1:B:9:ASN:HD22	1:B:10:TYR:N	2.13	0.47
2:B:803:4LG:H10	2:B:803:4LG:H241	1.76	0.46
1:B:128:ILE:CG1	1:B:137:PRO:HD3	2.43	0.46
1:A:151:ASP:HB3	1:A:323:ARG:HB2	1.97	0.46
1:B:15:TYR:O	1:B:31:VAL:HG22	2.16	0.46
1:B:185:TYR:CD2	1:B:326:ARG:HG3	2.50	0.46
1:A:294:HIS:HD2	1:A:294:HIS:O	1.98	0.46
1:A:44:SER:HA	1:A:58:LEU:HB3	1.97	0.46
1:B:89:GLN:HE21	1:B:102:MET:HE3	1.81	0.46
1:A:189:ILE:CD1	1:A:215:LEU:HG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:O	1:B:83:VAL:HG13	2.16	0.46
1:A:226:SER:OG	1:A:307:ALA:HB3	2.15	0.45
1:A:150:GLU:C	1:A:152:VAL:H	2.20	0.45
1:A:154:SER:HB2	1:A:317:TYR:OH	2.17	0.45
1:B:142:ILE:O	1:B:145:GLN:HG2	2.16	0.45
1:B:200:GLY:HA2	1:B:210:CYS:O	2.16	0.45
1:B:272:LEU:HD23	1:B:276:ASP:CB	2.46	0.45
1:B:133:GLY:O	1:B:134:ARG:HB3	2.16	0.45
1:A:255:GLY:O	1:A:258:LEU:HG	2.17	0.45
1:B:87:LEU:CD2	1:B:135:VAL:HG21	2.45	0.45
1:B:50:TYR:O	1:B:51:THR:C	2.54	0.45
1:B:112:LEU:HA	1:B:113:PRO:HA	1.67	0.45
1:A:9:ASN:HD21	1:A:12:ASP:HA	1.82	0.44
1:A:44:SER:HA	1:A:58:LEU:HD13	2.00	0.44
1:B:78:TYR:N	1:B:81:GLY:HA3	2.32	0.44
1:B:64:SER:HB3	1:B:67:TYR:HB2	2.00	0.44
1:A:77:ARG:HA	1:A:82:THR:H	1.82	0.44
1:B:78:TYR:HE2	1:B:113:PRO:HD3	1.83	0.44
1:A:327:ILE:HG22	1:A:329:PHE:CE1	2.52	0.44
1:A:268:LYS:NZ	1:A:269:GLU:HB2	2.33	0.44
1:A:196:ILE:HD12	1:A:265:LEU:HD22	1.98	0.44
1:B:215:LEU:HB2	1:B:305:THR:HG22	1.97	0.44
1:B:5:VAL:HG13	1:B:5:VAL:O	2.17	0.44
1:A:106:VAL:HG11	1:A:109:MET:CG	2.48	0.44
1:B:6:ILE:N	1:B:6:ILE:HD12	2.32	0.44
1:A:250:VAL:O	1:A:251:LYS:C	2.54	0.44
1:A:218:VAL:HG21	1:A:327:ILE:HD13	2.00	0.44
1:A:32:PHE:HB2	1:A:169:ILE:HD11	1.99	0.44
1:B:50:TYR:CZ	1:B:108:GLU:CB	3.01	0.44
1:B:156:TYR:HB2	1:B:317:TYR:CE2	2.53	0.44
1:A:134:ARG:NH2	1:A:134:ARG:HB2	2.32	0.44
1:B:255:GLY:HA3	1:B:280:GLN:HE22	1.82	0.44
1:A:225:ILE:HD11	1:A:272:LEU:HD11	1.99	0.44
1:A:171:LEU:N	1:A:171:LEU:HD22	2.32	0.44
1:B:69:HIS:ND1	1:B:70:ASN:N	2.66	0.43
1:A:138:ILE:HG23	1:A:139:PHE:N	2.34	0.43
1:B:232:ILE:O	1:B:236:MET:HG2	2.18	0.43
1:A:250:VAL:HG13	1:A:251:LYS:O	2.19	0.43
1:B:245:LEU:HD23	1:B:246:PHE:HB3	2.01	0.43
1:B:222:ALA:O	2:B:803:4LG:H191	2.17	0.43
1:B:109:MET:HA	1:B:110:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HB3	1:B:89:GLN:HB3	2.00	0.43
1:A:12:ASP:OD2	1:A:160:ASP:HB2	2.19	0.43
1:A:80:THR:O	1:A:81:GLY:O	2.36	0.43
1:A:81:GLY:O	1:A:82:THR:HB	2.18	0.43
1:B:128:ILE:HA	1:B:137:PRO:HG2	2.00	0.43
1:B:145:GLN:O	1:B:147:VAL:HG13	2.18	0.43
1:A:160:ASP:OD2	1:A:161:SER:N	2.50	0.43
1:B:151:ASP:HB3	1:B:323:ARG:HB2	2.00	0.43
1:B:10:TYR:CG	1:B:118:GLU:HG3	2.54	0.43
1:B:40:TRP:CB	2:B:803:4LG:H321	2.49	0.43
1:B:217:LEU:CD2	1:B:219:ASP:HB2	2.43	0.43
1:A:85:GLY:HA3	1:A:105:GLU:O	2.18	0.43
1:B:232:ILE:HG22	1:B:232:ILE:O	2.19	0.43
1:B:290:THR:CG2	1:B:291:LEU:N	2.82	0.43
1:A:236:MET:HG3	1:A:248:TYR:CZ	2.53	0.43
1:B:70:ASN:O	1:B:87:LEU:O	2.37	0.43
1:A:85:GLY:HA2	1:A:107:THR:OG1	2.19	0.42
1:A:110:PRO:HG2	1:A:114:PHE:HE1	1.84	0.42
1:A:223:SER:HA	2:A:804:4LG:H192	2.00	0.42
1:B:50:TYR:C	1:B:52:ALA:N	2.70	0.42
1:B:79:SER:O	1:B:80:THR:HB	2.19	0.42
1:B:122:VAL:HG23	2:B:803:4LG:C1	2.49	0.42
1:A:290:THR:CG2	1:A:291:LEU:N	2.82	0.42
1:A:290:THR:HG22	1:A:291:LEU:N	2.34	0.42
1:A:236:MET:SD	1:A:248:TYR:CG	3.12	0.42
1:A:194:TRP:CH2	1:A:320:PHE:HB3	2.55	0.42
1:A:40:TRP:CZ2	1:A:132:ILE:HD12	2.54	0.42
1:A:239:LEU:CD2	1:A:259:PRO:HG2	2.48	0.42
1:B:225:ILE:HG13	1:B:311:THR:HB	2.02	0.42
1:B:305:THR:HB	1:B:306:TRP:H	1.19	0.42
1:A:324:ASN:O	1:A:326:ARG:HG3	2.20	0.42
1:B:232:ILE:HG13	1:B:295:ALA:HA	2.00	0.42
1:A:61:ALA:HB1	1:A:67:TYR:CD1	2.55	0.42
1:B:13:THR:O	1:B:223:SER:OG	2.38	0.42
1:A:38:ASN:ND2	1:A:132:ILE:H	2.13	0.42
1:B:245:LEU:CD2	1:B:246:PHE:CB	2.96	0.42
1:A:268:LYS:HA	1:A:268:LYS:HD2	1.70	0.42
1:B:191:THR:CG2	1:B:192:GLY:N	2.83	0.42
1:A:83:VAL:HG21	2:A:804:4LG:H322	2.02	0.42
1:B:102:MET:HB3	1:B:135:VAL:HG11	2.01	0.42
1:A:294:HIS:C	1:A:294:HIS:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLN:HA	1:A:177:GLN:NE2	2.35	0.42
1:A:150:GLU:C	1:A:152:VAL:N	2.73	0.41
1:B:199:LYS:HZ2	1:B:266:GLY:HA2	1.81	0.41
1:A:44:SER:HA	1:A:58:LEU:CD1	2.50	0.41
1:A:99:VAL:HG12	1:A:145:GLN:OE1	2.20	0.41
1:A:228:SER:O	1:A:232:ILE:HG12	2.19	0.41
1:B:134:ARG:O	1:B:134:ARG:HG2	2.20	0.41
1:A:53:CYS:O	1:A:54:VAL:HG23	2.20	0.41
1:A:76:LEU:CD1	1:A:83:VAL:HG22	2.50	0.41
1:B:9:ASN:ND2	1:B:9:ASN:C	2.73	0.41
1:B:201:VAL:CG2	1:B:209:LEU:CB	2.98	0.41
1:B:7:LEU:HB2	1:B:167:GLY:CA	2.50	0.41
1:B:16:TYR:HB3	1:B:31:VAL:HG23	2.02	0.41
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.83	0.41
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.81	0.41
1:A:42:PRO:HB2	1:A:58:LEU:CD2	2.50	0.41
1:B:299:PRO:HA	1:B:300:PRO:HD3	1.86	0.41
1:A:81:GLY:O	1:A:82:THR:CG2	2.67	0.41
1:A:139:PHE:CE1	1:A:143:ILE:HD11	2.55	0.41
1:B:48:ARG:C	1:B:50:TYR:H	2.23	0.41
1:B:245:LEU:CG	1:B:246:PHE:N	2.83	0.41
1:B:117:ALA:HB3	2:B:803:4LG:H5	2.01	0.41
1:A:236:MET:HG3	1:A:248:TYR:CE1	2.55	0.41
1:B:77:ARG:N	1:B:77:ARG:HD2	2.35	0.41
1:B:212:ASP:N	1:B:212:ASP:OD2	2.54	0.41
2:A:804:4LG:H241	2:A:804:4LG:H10	1.84	0.41
1:A:103:PHE:N	1:A:103:PHE:CD1	2.89	0.41
1:A:109:MET:HE2	2:A:804:4LG:H8	2.03	0.41
1:B:50:TYR:O	1:B:52:ALA:N	2.54	0.41
1:B:236:MET:HG3	1:B:248:TYR:CG	2.56	0.41
1:B:242:LYS:O	1:B:248:TYR:HA	2.21	0.41
1:A:201:VAL:HG21	1:A:306:TRP:CZ2	2.56	0.41
1:A:168:GLN:HG2	1:A:169:ILE:N	2.36	0.41
1:A:190:LYS:O	1:A:191:THR:C	2.59	0.41
1:A:207:THR:HG22	1:A:207:THR:O	2.21	0.41
1:A:9:ASN:HD21	1:A:12:ASP:CA	2.35	0.40
1:B:128:ILE:O	1:B:128:ILE:HG12	2.21	0.40
1:B:264:HIS:O	1:B:265:LEU:HD23	2.21	0.40
1:A:225:ILE:HA	1:A:307:ALA:O	2.21	0.40
1:B:40:TRP:HZ2	1:B:76:LEU:HD21	1.86	0.40
1:A:127:PHE:CD2	1:A:322:ARG:NH1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:N	1:A:210:CYS:SG	2.87	0.40
1:B:186:ILE:HG21	1:B:196:ILE:HD12	2.03	0.40
1:B:143:ILE:HD13	1:B:148:LEU:HD12	2.02	0.40
1:B:317:TYR:N	1:B:332:ALA:HB2	2.36	0.40
1:A:34:THR:HA	1:A:125:MET:HB2	2.04	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	324/333 (97%)	270 (83%)	37 (11%)	17 (5%)	2 8
1	B	324/333 (97%)	287 (89%)	28 (9%)	9 (3%)	6 24
All	All	648/666 (97%)	557 (86%)	65 (10%)	26 (4%)	4 15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	80	THR
1	A	81	GLY
1	A	82	THR
1	A	83	VAL
1	A	212	ASP
1	A	295	ALA
1	B	83	VAL
1	A	209	LEU
1	B	70	ASN
1	B	79	SER
1	B	213	GLY
1	A	296	MET

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Mol	Chain	Res	Type
1	B	80	THR
1	B	114	PHE
1	B	206	SER
1	B	266	GLY
1	A	12	ASP
1	A	54	VAL
1	A	189	ILE
1	A	236	MET
1	A	292	ALA
1	A	110	PRO
1	A	256	PRO
1	A	213	GLY
1	B	138	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	A	279/284 (98%)	256 (92%)	23 (8%)	14 39
1	B	279/284 (98%)	249 (89%)	30 (11%)	8 24
All	All	558/568 (98%)	505 (90%)	53 (10%)	11 31

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	40	TRP
1	A	51	THR
1	A	76	LEU
1	A	77	ARG
1	A	87	LEU
1	A	94	VAL
1	A	106	VAL
1	A	158	ASN
1	A	199	LYS

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Mol	Chain	Res	Type
1	A	208	LEU
1	A	217	LEU
1	A	237	GLU
1	A	245	LEU
1	A	250	VAL
1	A	251	LYS
1	A	273	THR
1	A	278	VAL
1	A	280	GLN
1	A	294	HIS
1	A	297	ASP
1	A	326	ARG
1	A	331	LEU
1	B	9	ASN
1	B	18	GLU
1	B	31	VAL
1	B	51	THR
1	B	77	ARG
1	B	102	MET
1	B	115	MET
1	B	140	ASP
1	B	190	LYS
1	B	208	LEU
1	B	212	ASP
1	B	217	LEU
1	B	223	SER
1	B	224	TYR
1	B	237	GLU
1	B	239	LEU
1	B	243	LYS
1	B	245	LEU
1	B	246	PHE
1	B	250	VAL
1	B	258	LEU
1	B	272	LEU
1	B	282	SER
1	B	286	LYS
1	B	291	LEU
1	B	305	THR
1	B	315	LYS
1	B	323	ARG
1	B	325	ASN

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Mol	Chain	Res	Type
1	B	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	38	ASN
1	A	101	GLN
1	A	130	GLN
1	A	141	ASN
1	A	145	GLN
1	A	158	ASN
1	A	168	GLN
1	A	177	GLN
1	A	264	HIS
1	A	294	HIS
1	B	9	ASN
1	B	26	GLN
1	B	89	GLN
1	B	101	GLN
1	B	168	GLN
1	B	280	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

2 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	$\#\|Z\| > 2$
2	4LG	A	804	-	46,47,47	1.94	11 (23%)	50,63,63	2.31	10 (20%)
2	4LG	B	803	-	46,47,47	2.05	12 (26%)	50,63,63	2.40	13 (26%)

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
2	4LG	A	804	-	-	0/26/40/40	0/5/5/5
2	4LG	B	803	-	-	0/26/40/40	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	4LG	C11-N1	-5.17	1.33	1.39
2	A	804	4LG	C11-N1	-3.67	1.35	1.39
2	B	803	4LG	C10-C11	-3.02	1.34	1.40
2	B	803	4LG	C17-C18	-2.71	1.46	1.52
2	A	804	4LG	C17-C18	-2.68	1.46	1.52
2	A	804	4LG	C10-C11	-2.58	1.35	1.40
2	A	804	4LG	C21-N2	-2.10	1.43	1.46
2	B	803	4LG	C25-C26	2.00	1.43	1.39
2	A	804	4LG	C28-C27	2.05	1.42	1.38
2	A	804	4LG	C28-C29	2.09	1.42	1.38
2	B	803	4LG	C28-C27	2.13	1.42	1.38
2	B	803	4LG	C28-C29	2.22	1.43	1.38
2	B	803	4LG	C27-C26	2.22	1.43	1.39
2	A	804	4LG	C27-C26	2.46	1.44	1.39
2	A	804	4LG	C23-N3	2.54	1.41	1.36
2	B	803	4LG	C14-C9	2.85	1.44	1.38
2	A	804	4LG	C14-C9	2.99	1.44	1.38
2	B	803	4LG	O1-C2	3.24	1.42	1.37
2	B	803	4LG	C23-N3	3.31	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	804	4LG	C13-C14	3.93	1.44	1.36
2	B	803	4LG	C13-C14	4.20	1.45	1.36
2	B	803	4LG	C22-C23	6.57	1.56	1.51
2	A	804	4LG	C22-C23	7.47	1.57	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	804	4LG	O1-C2-C5	-4.56	116.67	124.35
2	B	803	4LG	O1-C2-C5	-3.91	117.77	124.35
2	B	803	4LG	O5-C23-C22	-2.61	115.10	120.32
2	B	803	4LG	C14-C9-C10	-2.56	117.16	120.84
2	A	804	4LG	C14-C9-C10	-2.26	117.59	120.84
2	B	803	4LG	C16-C12-C11	-2.25	104.28	106.20
2	A	804	4LG	C16-C12-C11	-2.20	104.32	106.20
2	A	804	4LG	O5-C23-C22	-2.11	116.11	120.32
2	B	803	4LG	C4-C3-C2	-2.01	117.20	120.47
2	A	804	4LG	O5-C23-N3	2.11	124.36	122.61
2	B	803	4LG	O5-C23-N3	2.18	124.42	122.61
2	B	803	4LG	C27-C26-N3	2.45	122.95	120.11
2	B	803	4LG	C22-C23-N3	2.55	120.48	116.46
2	A	804	4LG	C4-O2-C33	2.95	121.75	112.80
2	B	803	4LG	O2-C4-C3	3.08	119.88	109.77
2	A	804	4LG	C9-C10-C11	3.28	123.35	117.25
2	B	803	4LG	C9-C10-C11	3.61	123.95	117.25
2	B	803	4LG	O1-C2-C3	5.46	122.83	115.83
2	A	804	4LG	O1-C2-C3	6.17	123.75	115.83
2	A	804	4LG	C17-N1-C15	7.19	136.68	124.78
2	B	803	4LG	C17-N1-C15	7.82	137.71	124.78
2	A	804	4LG	O6-C24-C20	8.52	121.69	107.81
2	B	803	4LG	O6-C24-C20	8.62	121.84	107.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	4LG	9	0
2	B	803	4LG	12	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	328/333 (98%)	1.03	38 (11%) 6 4	22, 49, 83, 98	0
1	B	328/333 (98%)	0.65	16 (4%) 33 27	21, 40, 64, 78	0
All	All	656/666 (98%)	0.84	54 (8%) 14 9	21, 43, 78, 98	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	SER	6.1
1	A	208	LEU	5.8
1	A	203	VAL	5.8
1	A	205	SER	4.8
1	A	209	LEU	4.7
1	A	82	THR	4.5
1	A	201	VAL	4.3
1	A	202	SER	4.2
1	A	261	ILE	3.8
1	A	207	THR	3.5
1	A	71	GLY	3.4
1	A	294	HIS	3.3
1	A	234	LYS	3.1
1	B	216	ALA	3.1
1	A	325	ASN	3.1
1	A	281	GLU	3.0
1	B	74	LEU	3.0
1	A	49	LEU	2.9
1	B	78	TYR	2.8
1	A	236	MET	2.8
1	A	147	VAL	2.8
1	B	298	ILE	2.7
1	A	93	THR	2.6
1	A	173	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	272	LEU	2.5
1	B	238	ALA	2.5
1	B	246	PHE	2.5
1	B	81	GLY	2.5
1	B	248	TYR	2.5
1	A	277	TYR	2.4
1	B	48	ARG	2.4
1	A	263	PHE	2.4
1	B	235	LEU	2.4
1	A	286	LYS	2.3
1	A	227	GLY	2.2
1	A	306	TRP	2.2
1	A	150	GLU	2.2
1	A	184	HIS	2.2
1	B	184	HIS	2.2
1	B	76	LEU	2.2
1	A	148	LEU	2.1
1	A	161	SER	2.1
1	A	232	ILE	2.1
1	B	143	ILE	2.1
1	B	110	PRO	2.1
1	A	116	LEU	2.1
1	A	327	ILE	2.1
1	A	186	ILE	2.1
1	B	300	PRO	2.1
1	A	74	LEU	2.0
1	B	53	CYS	2.0
1	A	237	GLU	2.0
1	A	138	ILE	2.0
1	A	239	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 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, 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
2	4LG	A	804	43/43	0.85	0.30	0.86	33,39,47,49	0
2	4LG	B	803	43/43	0.81	0.29	0.57	24,36,43,44	0

6.5 Other polymers

There are no such residues in this entry.