Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:15 PM GMT

PDB ID	:	1JHN
Title	:	Crystal Structure of the Lumenal Domain of Calnexin
Authors	:	Schrag, J.D.; Bergeron, J.M.; Li, Y.; Borisova, S.; Hahn, M.; Thomas, D.Y.; Cygler, M.
Deposited on	:	2001-06-28
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:

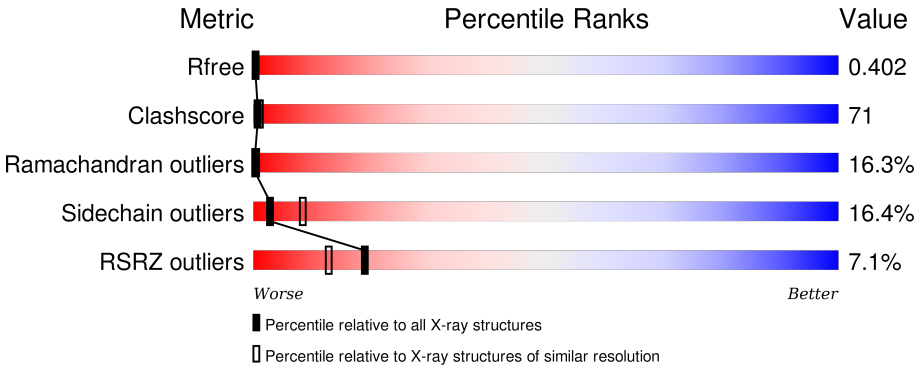
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
R_{free}	91344	1451 (2.90-2.90)
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	424	6%, 22%, 49%, 16%, •, 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2854 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 calnexin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	2853	1819	466	555	13	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

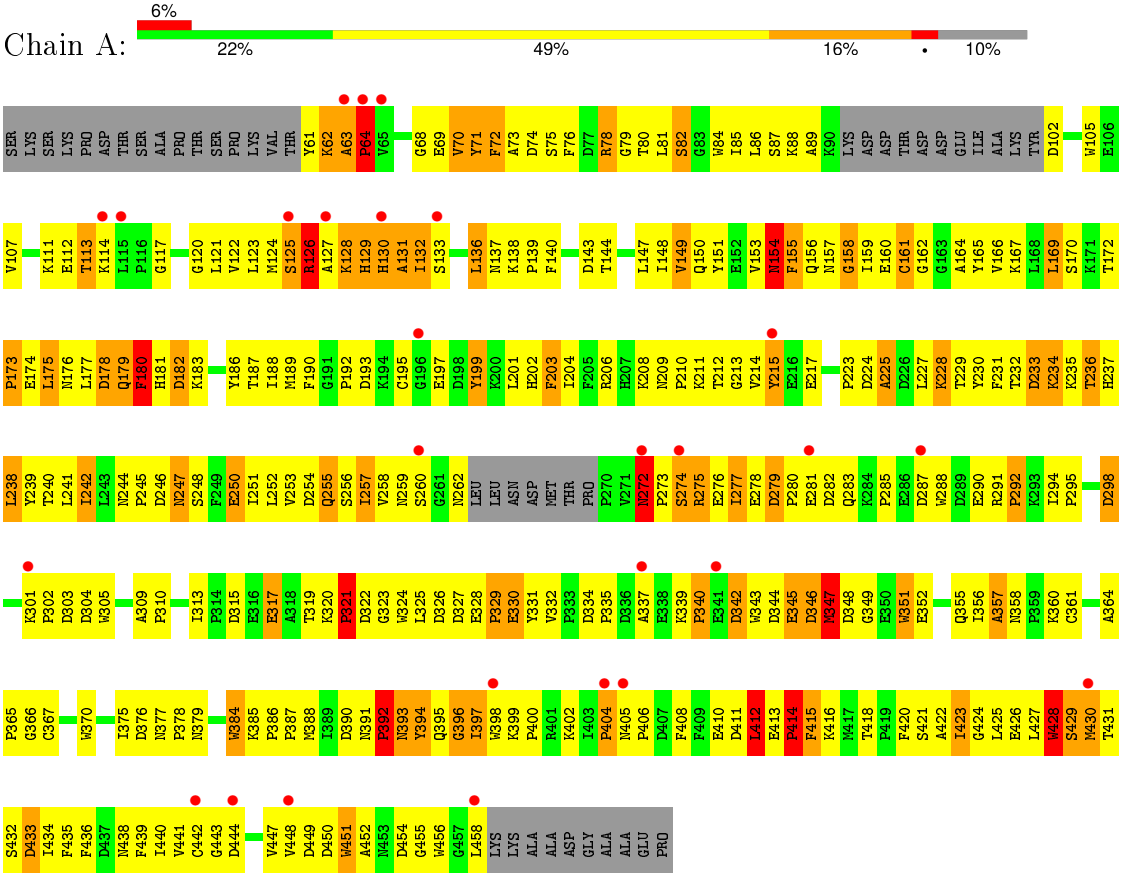
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0

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: calnexin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.77Å 85.77Å 143.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.80 – 2.90 33.83 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.80-2.90) 99.6 (33.83-2.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.15 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.327 , 0.377 0.345 , 0.402	Depositor DCC
R_{free} test set	590 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 12312 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	2854	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

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	0.54	0/2948	0.75	0/4046

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	2853	0	2454	374	0
2	A	1	0	0	0	0
All	All	2854	0	2454	374	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 71.

All (374) 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:301:LYS:HE3	1:A:384:TRP:HB2	1.36	1.07
1:A:123:LEU:HD12	1:A:124:MET:H	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:OG1	1:A:173:PRO:HD2	1.63	0.97
1:A:248:SER:HA	1:A:262:ASN:HA	1.47	0.96
1:A:159:ILE:HD11	1:A:231:PHE:HB3	1.47	0.93
1:A:154:ASN:C	1:A:154:ASN:HD22	1.75	0.91
1:A:347:MET:C	1:A:349:GLY:H	1.74	0.91
1:A:276:GLU:HG2	1:A:277:ILE:H	1.38	0.88
1:A:201:LEU:HD21	1:A:251:ILE:HG21	1.56	0.88
1:A:84:TRP:HB3	1:A:132:ILE:HD11	1.53	0.88
1:A:164:ALA:HA	1:A:427:LEU:HD13	1.56	0.85
1:A:71:TYR:N	1:A:137:ASN:HD21	1.76	0.84
1:A:181:HIS:NE2	1:A:183:LYS:HB2	1.92	0.84
1:A:391:ASN:O	1:A:393:ASN:N	2.10	0.84
1:A:173:PRO:HG2	1:A:174:GLU:H	1.44	0.83
1:A:233:ASP:O	1:A:235:LYS:N	2.12	0.82
1:A:71:TYR:H	1:A:137:ASN:HD21	1.26	0.82
1:A:332:VAL:HG13	1:A:358:ASN:HB2	1.61	0.81
1:A:148:ILE:HG13	1:A:242:ILE:HG23	1.63	0.81
1:A:167:LYS:HD2	1:A:186:TYR:CD2	2.15	0.80
1:A:154:ASN:HB2	1:A:236:THR:HA	1.64	0.80
1:A:250:GLU:HB2	1:A:257:ILE:HG23	1.64	0.79
1:A:147:LEU:C	1:A:148:ILE:HD12	2.03	0.79
1:A:242:ILE:N	1:A:242:ILE:HD12	1.99	0.78
1:A:153:VAL:HA	1:A:435:PHE:O	1.83	0.77
1:A:295:PRO:HA	1:A:388:MET:HE2	1.67	0.76
1:A:107:VAL:O	1:A:107:VAL:HG12	1.86	0.76
1:A:412:LEU:C	1:A:414:PRO:HD3	2.04	0.76
1:A:153:VAL:HG12	1:A:239:TYR:CE1	2.20	0.76
1:A:149:VAL:HG13	1:A:241:LEU:HB3	1.68	0.75
1:A:81:LEU:H	1:A:81:LEU:HD23	1.50	0.75
1:A:275:ARG:HH11	1:A:275:ARG:HA	1.51	0.75
1:A:105:TRP:CE3	1:A:121:LEU:HD21	2.22	0.74
1:A:87:SER:O	1:A:88:LYS:HD3	1.87	0.74
1:A:323:GLY:O	1:A:365:PRO:HD2	1.88	0.74
1:A:127:ALA:O	1:A:128:LYS:HB2	1.88	0.73
1:A:201:LEU:HD21	1:A:251:ILE:CG2	2.19	0.72
1:A:390:ASP:O	1:A:392:PRO:HD3	1.89	0.72
1:A:209:ASN:HB3	1:A:214:VAL:N	2.04	0.72
1:A:153:VAL:HG12	1:A:239:TYR:HE1	1.53	0.72
1:A:64:PRO:HG3	1:A:454:ASP:C	2.10	0.72
1:A:148:ILE:HB	1:A:442:CYS:O	1.91	0.70
1:A:123:LEU:HD12	1:A:124:MET:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HB3	1:A:451:TRP:HH2	1.57	0.69
1:A:80:THR:C	1:A:82:SER:H	1.94	0.69
1:A:423:ILE:HG23	1:A:423:ILE:O	1.90	0.69
1:A:294:ILE:HB	1:A:295:PRO:HD2	1.75	0.69
1:A:274:SER:O	1:A:275:ARG:HD2	1.91	0.69
1:A:181:HIS:CE1	1:A:183:LYS:H	2.10	0.68
1:A:154:ASN:C	1:A:154:ASN:ND2	2.46	0.68
1:A:154:ASN:O	1:A:154:ASN:ND2	2.26	0.68
1:A:84:TRP:HB3	1:A:132:ILE:CD1	2.21	0.67
1:A:347:MET:C	1:A:349:GLY:N	2.40	0.67
1:A:276:GLU:HG2	1:A:277:ILE:N	2.08	0.67
1:A:399:LYS:HE2	1:A:400:PRO:HD2	1.76	0.67
1:A:242:ILE:H	1:A:242:ILE:HD12	1.57	0.67
1:A:177:LEU:O	1:A:180:PHE:N	2.28	0.67
1:A:208:LYS:O	1:A:210:PRO:HD3	1.94	0.67
1:A:340:PRO:C	1:A:342:ASP:H	1.97	0.67
1:A:255:GLN:N	1:A:255:GLN:HE21	1.93	0.66
1:A:68:GLY:H	1:A:447:VAL:HG13	1.61	0.66
1:A:203:PHE:C	1:A:203:PHE:CD1	2.65	0.66
1:A:154:ASN:OD1	1:A:236:THR:N	2.29	0.66
1:A:405:ASN:ND2	1:A:408:PHE:HA	2.11	0.66
1:A:209:ASN:HB3	1:A:214:VAL:H	1.61	0.66
1:A:161:CYS:CB	1:A:195:CYS:HG	2.09	0.65
1:A:136:LEU:HG	1:A:421:SER:C	2.16	0.65
1:A:328:GLU:OE1	1:A:360:LYS:HD2	1.95	0.65
1:A:412:LEU:O	1:A:414:PRO:HD3	1.97	0.65
1:A:86:LEU:HD12	1:A:131:ALA:CB	2.27	0.64
1:A:250:GLU:HA	1:A:259:ASN:O	1.97	0.64
1:A:182:ASP:OD2	1:A:183:LYS:HD3	1.98	0.64
1:A:252:LEU:HA	1:A:257:ILE:HA	1.80	0.64
1:A:75:SER:HB3	1:A:451:TRP:CH2	2.33	0.64
1:A:203:PHE:C	1:A:203:PHE:HD1	2.00	0.64
1:A:384:TRP:HA	1:A:384:TRP:CE3	2.32	0.63
1:A:160:GLU:HB2	1:A:430:MET:HG2	1.80	0.63
1:A:330:GLU:HG3	1:A:331:TYR:CD1	2.34	0.63
1:A:87:SER:H	1:A:131:ALA:HB1	1.63	0.63
1:A:154:ASN:O	1:A:156:GLN:N	2.32	0.63
1:A:224:ASP:O	1:A:225:ALA:HB2	1.97	0.63
1:A:377:ASN:OD1	1:A:377:ASN:C	2.37	0.63
1:A:177:LEU:O	1:A:179:GLN:N	2.32	0.63
1:A:179:GLN:O	1:A:181:HIS:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:HE3	1:A:132:ILE:HG13	1.65	0.62
1:A:384:TRP:HA	1:A:384:TRP:HE3	1.64	0.62
1:A:223:PRO:HG3	1:A:259:ASN:HD22	1.63	0.62
1:A:148:ILE:HG21	1:A:448:VAL:HG21	1.80	0.61
1:A:150:GLN:HG3	1:A:239:TYR:O	2.00	0.61
1:A:175:LEU:HD23	1:A:175:LEU:H	1.65	0.61
1:A:394:TYR:O	1:A:394:TYR:CG	2.52	0.61
1:A:161:CYS:HG	1:A:195:CYS:HG	0.62	0.61
1:A:250:GLU:HB2	1:A:257:ILE:CG2	2.29	0.61
1:A:206:ARG:HA	1:A:217:GLU:HA	1.81	0.61
1:A:339:LYS:HB3	1:A:351:TRP:CG	2.36	0.61
1:A:394:TYR:O	1:A:394:TYR:CD2	2.54	0.61
1:A:136:LEU:HG	1:A:421:SER:O	2.01	0.61
1:A:375:ILE:HG13	1:A:376:ASP:O	2.00	0.61
1:A:173:PRO:HG2	1:A:174:GLU:N	2.16	0.60
1:A:161:CYS:HA	1:A:195:CYS:HA	1.81	0.60
1:A:285:PRO:HG2	1:A:288:TRP:HB2	1.84	0.60
1:A:209:ASN:O	1:A:213:GLY:HA2	2.02	0.60
1:A:147:LEU:HD12	1:A:148:ILE:H	1.66	0.60
1:A:223:PRO:HB3	1:A:259:ASN:HB2	1.83	0.60
1:A:143:ASP:CG	1:A:144:THR:H	2.04	0.60
1:A:162:GLY:HA3	1:A:429:SER:HA	1.84	0.60
1:A:250:GLU:HA	1:A:260:SER:HA	1.85	0.59
1:A:391:ASN:O	1:A:394:TYR:N	2.35	0.59
1:A:136:LEU:HD11	1:A:420:PHE:CD2	2.38	0.59
1:A:161:CYS:HB2	1:A:195:CYS:SG	2.43	0.59
1:A:136:LEU:HD11	1:A:420:PHE:CE2	2.38	0.59
1:A:172:THR:CB	1:A:173:PRO:HD2	2.31	0.59
1:A:253:VAL:O	1:A:254:ASP:HB2	2.03	0.59
1:A:157:ASN:O	1:A:158:GLY:O	2.21	0.59
1:A:179:GLN:O	1:A:179:GLN:NE2	2.36	0.58
1:A:147:LEU:HD12	1:A:148:ILE:N	2.18	0.58
1:A:398:TRP:O	1:A:399:LYS:HG2	2.02	0.58
1:A:395:GLN:O	1:A:396:GLY:O	2.20	0.58
1:A:68:GLY:O	1:A:447:VAL:HG11	2.03	0.58
1:A:129:HIS:O	1:A:131:ALA:N	2.36	0.58
1:A:238:LEU:HD23	1:A:254:ASP:H	1.68	0.58
1:A:229:THR:O	1:A:233:ASP:OD2	2.22	0.58
1:A:169:LEU:HD13	1:A:169:LEU:H	1.69	0.58
1:A:72:PHE:O	1:A:441:VAL:N	2.36	0.57
1:A:246:ASP:O	1:A:247:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:HB3	1:A:441:VAL:O	2.04	0.57
1:A:181:HIS:CG	1:A:182:ASP:N	2.73	0.57
1:A:394:TYR:CZ	1:A:396:GLY:HA2	2.40	0.57
1:A:291:ARG:NH2	1:A:294:ILE:HG21	2.20	0.57
1:A:84:TRP:CE3	1:A:132:ILE:HG13	2.40	0.57
1:A:202:HIS:HB3	1:A:204:ILE:CD1	2.34	0.57
1:A:391:ASN:C	1:A:393:ASN:H	2.08	0.56
1:A:217:GLU:O	1:A:217:GLU:HG3	2.05	0.56
1:A:175:LEU:O	1:A:177:LEU:N	2.38	0.56
1:A:169:LEU:O	1:A:420:PHE:HB2	2.06	0.56
1:A:410:GLU:CD	1:A:411:ASP:H	2.09	0.56
1:A:175:LEU:HD23	1:A:175:LEU:N	2.21	0.56
1:A:86:LEU:HD12	1:A:131:ALA:HB1	1.88	0.56
1:A:161:CYS:O	1:A:430:MET:HB2	2.06	0.55
1:A:148:ILE:N	1:A:148:ILE:HD12	2.21	0.55
1:A:73:ALA:HA	1:A:439:PHE:O	2.06	0.55
1:A:161:CYS:CB	1:A:195:CYS:SG	2.94	0.55
1:A:126:ARG:O	1:A:126:ARG:HD3	2.07	0.55
1:A:279:ASP:C	1:A:281:GLU:H	2.09	0.55
1:A:84:TRP:CB	1:A:132:ILE:HD11	2.29	0.55
1:A:387:PRO:O	1:A:388:MET:HE2	2.07	0.55
1:A:69:GLU:HG3	1:A:70:VAL:H	1.71	0.55
1:A:356:ILE:O	1:A:357:ALA:HB2	2.06	0.55
1:A:111:LYS:O	1:A:112:GLU:C	2.45	0.55
1:A:124:MET:O	1:A:125:SER:OG	2.21	0.55
1:A:398:TRP:C	1:A:399:LYS:HG2	2.28	0.55
1:A:181:HIS:ND1	1:A:182:ASP:N	2.50	0.55
1:A:159:ILE:HD11	1:A:231:PHE:CB	2.29	0.54
1:A:78:ARG:HD3	1:A:78:ARG:H	1.72	0.54
1:A:105:TRP:HE3	1:A:121:LEU:HD21	1.71	0.54
1:A:126:ARG:CZ	1:A:126:ARG:O	2.55	0.54
1:A:199:TYR:CD1	1:A:228:LYS:HA	2.42	0.54
1:A:317:GLU:OE1	1:A:317:GLU:HA	2.06	0.54
1:A:276:GLU:CG	1:A:277:ILE:N	2.70	0.54
1:A:413:GLU:O	1:A:415:PHE:N	2.40	0.54
1:A:140:PHE:C	1:A:140:PHE:CD1	2.80	0.54
1:A:190:PHE:CZ	1:A:241:LEU:HB2	2.43	0.53
1:A:273:PRO:HG3	1:A:411:ASP:CB	2.38	0.53
1:A:329:PRO:O	1:A:330:GLU:C	2.46	0.53
1:A:151:TYR:OH	1:A:165:TYR:HA	2.08	0.53
1:A:202:HIS:HB3	1:A:204:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLY:C	1:A:425:LEU:HD12	2.29	0.53
1:A:131:ALA:O	1:A:132:ILE:O	2.27	0.53
1:A:128:LYS:C	1:A:130:HIS:H	2.11	0.53
1:A:255:GLN:N	1:A:255:GLN:NE2	2.57	0.53
1:A:347:MET:SD	1:A:347:MET:C	2.88	0.52
1:A:76:PHE:HA	1:A:78:ARG:HE	1.73	0.52
1:A:282:ASP:OD1	1:A:283:GLN:N	2.42	0.52
1:A:291:ARG:HH21	1:A:294:ILE:HG21	1.72	0.52
1:A:182:ASP:HB2	1:A:426:GLU:OE2	2.09	0.52
1:A:181:HIS:CD2	1:A:183:LYS:H	2.27	0.52
1:A:169:LEU:HD13	1:A:169:LEU:N	2.25	0.52
1:A:414:PRO:O	1:A:416:LYS:N	2.43	0.52
1:A:276:GLU:HA	1:A:405:ASN:HB2	1.91	0.51
1:A:233:ASP:CG	1:A:237:HIS:HE2	2.14	0.51
1:A:204:ILE:N	1:A:204:ILE:HD12	2.25	0.51
1:A:399:LYS:HE2	1:A:399:LYS:HA	1.91	0.51
1:A:272:ASN:N	1:A:272:ASN:OD1	2.44	0.51
1:A:71:TYR:CB	1:A:441:VAL:O	2.59	0.51
1:A:105:TRP:HZ2	1:A:129:HIS:O	1.93	0.51
1:A:80:THR:C	1:A:82:SER:N	2.63	0.51
1:A:423:ILE:O	1:A:423:ILE:CG2	2.58	0.51
1:A:224:ASP:O	1:A:225:ALA:CB	2.59	0.51
1:A:70:VAL:HB	1:A:137:ASN:ND2	2.26	0.51
1:A:203:PHE:HD1	1:A:204:ILE:N	2.09	0.51
1:A:315:ASP:HB2	1:A:375:ILE:HG23	1.93	0.51
1:A:126:ARG:NH1	1:A:428:TRP:CH2	2.79	0.51
1:A:74:ASP:C	1:A:74:ASP:OD1	2.49	0.51
1:A:208:LYS:O	1:A:210:PRO:CD	2.59	0.50
1:A:153:VAL:HG11	1:A:192:PRO:HG3	1.93	0.50
1:A:215:TYR:OH	1:A:418:THR:HG21	2.10	0.50
1:A:340:PRO:C	1:A:342:ASP:N	2.63	0.50
1:A:126:ARG:CD	1:A:126:ARG:O	2.59	0.50
1:A:450:ASP:O	1:A:452:ALA:N	2.44	0.50
1:A:290:GLU:OE2	1:A:397:ILE:HD12	2.12	0.50
1:A:442:CYS:HB3	1:A:448:VAL:CG2	2.41	0.50
1:A:281:GLU:OE1	1:A:281:GLU:HA	2.12	0.50
1:A:332:VAL:HG22	1:A:358:ASN:N	2.26	0.50
1:A:242:ILE:N	1:A:242:ILE:CD1	2.65	0.50
1:A:107:VAL:HA	1:A:120:GLY:O	2.12	0.49
1:A:248:SER:CA	1:A:262:ASN:HA	2.30	0.49
1:A:325:LEU:CB	1:A:328:GLU:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HH11	1:A:275:ARG:CA	2.22	0.49
1:A:73:ALA:HA	1:A:440:ILE:HA	1.94	0.49
1:A:450:ASP:C	1:A:452:ALA:N	2.65	0.49
1:A:71:TYR:N	1:A:137:ASN:ND2	2.52	0.49
1:A:71:TYR:O	1:A:72:PHE:HB2	2.13	0.49
1:A:223:PRO:HB3	1:A:258:VAL:O	2.11	0.49
1:A:278:GLU:O	1:A:280:PRO:HD3	2.12	0.49
1:A:406:PRO:C	1:A:408:PHE:H	2.15	0.49
1:A:150:GLN:NE2	1:A:238:LEU:HD11	2.28	0.49
1:A:209:ASN:OD1	1:A:212:THR:N	2.46	0.49
1:A:227:LEU:O	1:A:228:LYS:C	2.50	0.49
1:A:126:ARG:NE	1:A:126:ARG:O	2.46	0.49
1:A:201:LEU:O	1:A:201:LEU:HG	2.12	0.48
1:A:393:ASN:N	1:A:393:ASN:ND2	2.61	0.48
1:A:250:GLU:N	1:A:250:GLU:OE1	2.47	0.48
1:A:107:VAL:O	1:A:107:VAL:CG1	2.56	0.48
1:A:343:TRP:CZ2	1:A:351:TRP:N	2.81	0.48
1:A:250:GLU:N	1:A:250:GLU:CD	2.66	0.48
1:A:251:ILE:O	1:A:253:VAL:HG23	2.13	0.48
1:A:64:PRO:HG3	1:A:454:ASP:O	2.13	0.48
1:A:303:ASP:N	1:A:303:ASP:OD1	2.46	0.48
1:A:346:ASP:C	1:A:347:MET:HG3	2.34	0.48
1:A:169:LEU:CD1	1:A:169:LEU:N	2.77	0.48
1:A:272:ASN:CG	1:A:273:PRO:HD2	2.34	0.48
1:A:127:ALA:O	1:A:428:TRP:HZ3	1.96	0.48
1:A:339:LYS:HB3	1:A:351:TRP:CD2	2.49	0.47
1:A:325:LEU:HB3	1:A:328:GLU:HB2	1.95	0.47
1:A:320:LYS:HD2	1:A:370:TRP:HB2	1.96	0.47
1:A:150:GLN:CD	1:A:238:LEU:HD11	2.34	0.47
1:A:133:SER:HA	1:A:424:GLY:HA2	1.96	0.47
1:A:86:LEU:HG	1:A:87:SER:O	2.14	0.47
1:A:442:CYS:SG	1:A:443:GLY:N	2.87	0.47
1:A:153:VAL:HG22	1:A:154:ASN:N	2.29	0.47
1:A:279:ASP:C	1:A:281:GLU:N	2.67	0.47
1:A:328:GLU:OE1	1:A:358:ASN:ND2	2.39	0.47
1:A:203:PHE:CD2	1:A:241:LEU:HD21	2.50	0.47
1:A:181:HIS:NE2	1:A:183:LYS:CB	2.72	0.47
1:A:276:GLU:CG	1:A:277:ILE:H	2.07	0.47
1:A:447:VAL:O	1:A:450:ASP:OD1	2.33	0.47
1:A:393:ASN:O	1:A:395:GLN:N	2.48	0.47
1:A:170:SER:HA	1:A:420:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:TRP:O	1:A:386:PRO:HD3	2.16	0.46
1:A:414:PRO:C	1:A:416:LYS:N	2.67	0.46
1:A:80:THR:CB	1:A:82:SER:OG	2.63	0.46
1:A:62:LYS:HD3	1:A:117:GLY:HA3	1.98	0.46
1:A:377:ASN:OD1	1:A:379:ASN:N	2.48	0.46
1:A:63:ALA:N	1:A:64:PRO:HD2	2.31	0.46
1:A:153:VAL:HG22	1:A:154:ASN:H	1.80	0.46
1:A:344:ASP:O	1:A:346:ASP:N	2.48	0.46
1:A:395:GLN:H	1:A:395:GLN:HG2	1.52	0.46
1:A:148:ILE:HD13	1:A:443:GLY:C	2.36	0.46
1:A:189:MET:HG2	1:A:190:PHE:N	2.31	0.46
1:A:173:PRO:CG	1:A:174:GLU:N	2.77	0.46
1:A:121:LEU:HD23	1:A:122:VAL:N	2.30	0.46
1:A:245:PRO:HA	1:A:415:PHE:CG	2.51	0.46
1:A:209:ASN:OD1	1:A:211:LYS:N	2.46	0.45
1:A:121:LEU:C	1:A:121:LEU:HD23	2.36	0.45
1:A:161:CYS:O	1:A:161:CYS:SG	2.74	0.45
1:A:391:ASN:C	1:A:393:ASN:N	2.69	0.45
1:A:233:ASP:O	1:A:234:LYS:C	2.53	0.45
1:A:244:ASN:C	1:A:246:ASP:N	2.70	0.45
1:A:63:ALA:HB3	1:A:64:PRO:CD	2.46	0.45
1:A:255:GLN:NE2	1:A:456:TRP:CZ3	2.85	0.45
1:A:246:ASP:O	1:A:247:ASN:CB	2.64	0.45
1:A:410:GLU:CD	1:A:411:ASP:N	2.70	0.45
1:A:244:ASN:C	1:A:246:ASP:H	2.20	0.45
1:A:320:LYS:O	1:A:321:PRO:O	2.34	0.45
1:A:345:GLU:O	1:A:347:MET:N	2.50	0.45
1:A:169:LEU:HB2	1:A:422:ALA:HB3	1.99	0.45
1:A:257:ILE:O	1:A:257:ILE:HG22	2.17	0.45
1:A:177:LEU:O	1:A:178:ASP:C	2.55	0.44
1:A:393:ASN:N	1:A:393:ASN:HD22	2.16	0.44
1:A:295:PRO:HA	1:A:387:PRO:O	2.17	0.44
1:A:313:ILE:HD11	1:A:378:PRO:HD2	1.98	0.44
1:A:324:TRP:CE3	1:A:366:GLY:HA3	2.53	0.44
1:A:112:GLU:O	1:A:113:THR:O	2.35	0.44
1:A:334:ASP:OD1	1:A:335:PRO:N	2.51	0.44
1:A:105:TRP:HE3	1:A:121:LEU:CD2	2.30	0.44
1:A:166:VAL:CG1	1:A:167:LYS:N	2.80	0.44
1:A:343:TRP:HE1	1:A:345:GLU:HA	1.83	0.44
1:A:70:VAL:C	1:A:72:PHE:H	2.19	0.44
1:A:255:GLN:CA	1:A:255:GLN:NE2	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:H	1:A:186:TYR:HA	1.83	0.44
1:A:344:ASP:O	1:A:345:GLU:C	2.55	0.44
1:A:87:SER:H	1:A:131:ALA:CB	2.31	0.44
1:A:412:LEU:HD12	1:A:414:PRO:CD	2.48	0.44
1:A:288:TRP:NE1	1:A:398:TRP:HB2	2.33	0.44
1:A:165:TYR:CD1	1:A:165:TYR:N	2.80	0.44
1:A:276:GLU:HG2	1:A:277:ILE:O	2.18	0.43
1:A:412:LEU:HB2	1:A:413:GLU:H	1.53	0.43
1:A:323:GLY:CA	1:A:365:PRO:HG2	2.48	0.43
1:A:377:ASN:OD1	1:A:378:PRO:N	2.51	0.43
1:A:217:GLU:CG	1:A:217:GLU:O	2.66	0.43
1:A:412:LEU:CD1	1:A:414:PRO:N	2.81	0.43
1:A:414:PRO:C	1:A:416:LYS:H	2.20	0.43
1:A:432:SER:OG	1:A:433:ASP:N	2.50	0.43
1:A:78:ARG:HG2	1:A:80:THR:H	1.84	0.43
1:A:399:LYS:HE2	1:A:400:PRO:CD	2.45	0.43
1:A:158:GLY:O	1:A:431:THR:HG21	2.19	0.43
1:A:238:LEU:HG	1:A:239:TYR:N	2.33	0.43
1:A:62:LYS:CD	1:A:117:GLY:HA3	2.48	0.43
1:A:434:ILE:HG22	1:A:436:PHE:CE1	2.54	0.43
1:A:84:TRP:O	1:A:85:ILE:HD13	2.18	0.43
1:A:72:PHE:CD1	1:A:72:PHE:C	2.91	0.43
1:A:444:ASP:OD1	1:A:447:VAL:N	2.41	0.43
1:A:324:TRP:CZ3	1:A:366:GLY:HA3	2.54	0.43
1:A:399:LYS:CE	1:A:399:LYS:HA	2.48	0.42
1:A:143:ASP:CG	1:A:144:THR:N	2.72	0.42
1:A:345:GLU:C	1:A:347:MET:N	2.72	0.42
1:A:233:ASP:C	1:A:235:LYS:N	2.71	0.42
1:A:392:PRO:HB2	1:A:393:ASN:ND2	2.34	0.42
1:A:438:ASN:HA	1:A:451:TRP:HZ2	1.84	0.42
1:A:181:HIS:CG	1:A:182:ASP:H	2.31	0.42
1:A:162:GLY:O	1:A:193:ASP:OD1	2.37	0.42
1:A:140:PHE:O	1:A:140:PHE:HD1	2.02	0.42
1:A:259:ASN:OD1	1:A:260:SER:N	2.53	0.42
1:A:255:GLN:NE2	1:A:456:TRP:HZ3	2.17	0.42
1:A:150:GLN:HB2	1:A:240:THR:HA	2.00	0.42
1:A:361:CYS:O	1:A:364:ALA:N	2.51	0.42
1:A:322:ASP:C	1:A:324:TRP:H	2.23	0.42
1:A:309:ALA:HA	1:A:310:PRO:HD3	1.85	0.42
1:A:346:ASP:O	1:A:347:MET:CB	2.67	0.42
1:A:351:TRP:CG	1:A:352:GLU:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:C	1:A:234:LYS:H	2.23	0.42
1:A:428:TRP:CE3	1:A:428:TRP:HA	2.55	0.42
1:A:278:GLU:CB	1:A:400:PRO:HB2	2.49	0.42
1:A:123:LEU:HD13	1:A:129:HIS:CB	2.50	0.42
1:A:355:GLN:HE21	1:A:355:GLN:HA	1.85	0.42
1:A:355:GLN:NE2	1:A:355:GLN:HA	2.35	0.42
1:A:251:ILE:HG22	1:A:251:ILE:O	2.19	0.42
1:A:332:VAL:CG1	1:A:358:ASN:HB2	2.43	0.42
1:A:291:ARG:O	1:A:292:PRO:C	2.58	0.42
1:A:412:LEU:CD1	1:A:414:PRO:HA	2.50	0.42
1:A:209:ASN:O	1:A:213:GLY:CA	2.67	0.42
1:A:291:ARG:HH21	1:A:294:ILE:CG2	2.33	0.41
1:A:334:ASP:HA	1:A:335:PRO:HD3	1.68	0.41
1:A:177:LEU:C	1:A:179:GLN:N	2.74	0.41
1:A:450:ASP:C	1:A:452:ALA:H	2.22	0.41
1:A:301:LYS:HB2	1:A:384:TRP:CG	2.55	0.41
1:A:396:GLY:O	1:A:397:ILE:C	2.59	0.41
1:A:148:ILE:HD13	1:A:443:GLY:HA2	2.02	0.41
1:A:223:PRO:CG	1:A:259:ASN:HD22	2.32	0.41
1:A:328:GLU:HA	1:A:329:PRO:HD2	1.68	0.41
1:A:187:THR:HG22	1:A:188:ILE:HG13	2.03	0.41
1:A:298:ASP:OD1	1:A:298:ASP:N	2.52	0.41
1:A:62:LYS:O	1:A:63:ALA:HB2	2.20	0.41
1:A:344:ASP:C	1:A:346:ASP:N	2.74	0.41
1:A:405:ASN:ND2	1:A:408:PHE:CA	2.81	0.41
1:A:159:ILE:HD12	1:A:159:ILE:O	2.20	0.41
1:A:209:ASN:C	1:A:211:LYS:H	2.24	0.41
1:A:328:GLU:HB3	1:A:367:CYS:SG	2.60	0.41
1:A:272:ASN:CG	1:A:273:PRO:CD	2.89	0.41
1:A:227:LEU:O	1:A:230:TYR:HD2	2.03	0.41
1:A:330:GLU:HG3	1:A:331:TYR:CE1	2.55	0.41
1:A:364:ALA:HA	1:A:365:PRO:HD3	1.94	0.41
1:A:78:ARG:HG2	1:A:79:GLY:N	2.36	0.41
1:A:279:ASP:O	1:A:281:GLU:N	2.54	0.41
1:A:138:LYS:HA	1:A:139:PRO:HD3	1.97	0.41
1:A:105:TRP:CE3	1:A:121:LEU:CD2	2.99	0.40
1:A:233:ASP:OD2	1:A:237:HIS:NE2	2.44	0.40
1:A:128:LYS:HG2	1:A:130:HIS:HB2	2.03	0.40
1:A:339:LYS:O	1:A:340:PRO:C	2.59	0.40
1:A:327:ASP:O	1:A:329:PRO:HD3	2.21	0.40
1:A:302:PRO:HG2	1:A:305:TRP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:O	1:A:256:SER:N	2.50	0.40
1:A:346:ASP:O	1:A:347:MET:HB3	2.22	0.40
1:A:320:LYS:HE3	1:A:326:ASP:OD1	2.20	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	374/424 (88%)	237 (63%)	76 (20%)	61 (16%)	0 0

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ALA
1	A	64	PRO
1	A	89	ALA
1	A	113	THR
1	A	126	ARG
1	A	128	LYS
1	A	130	HIS
1	A	132	ILE
1	A	155	PHE
1	A	158	GLY
1	A	178	ASP
1	A	180	PHE
1	A	225	ALA
1	A	228	LYS
1	A	234	LYS
1	A	247	ASN
1	A	272	ASN
1	A	330	GLU

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Mol	Chain	Res	Type
1	A	347	MET
1	A	357	ALA
1	A	392	PRO
1	A	396	GLY
1	A	404	PRO
1	A	412	LEU
1	A	414	PRO
1	A	62	LYS
1	A	70	VAL
1	A	72	PHE
1	A	114	LYS
1	A	125	SER
1	A	176	ASN
1	A	197	GLU
1	A	199	TYR
1	A	277	ILE
1	A	292	PRO
1	A	337	ALA
1	A	415	PHE
1	A	429	SER
1	A	129	HIS
1	A	173	PRO
1	A	257	ILE
1	A	346	ASP
1	A	394	TYR
1	A	451	TRP
1	A	455	GLY
1	A	131	ALA
1	A	136	LEU
1	A	154	ASN
1	A	321	PRO
1	A	351	TRP
1	A	402	LYS
1	A	430	MET
1	A	340	PRO
1	A	345	GLU
1	A	428	TRP
1	A	233	ASP
1	A	433	ASP
1	A	279	ASP
1	A	385	LYS
1	A	397	ILE

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Mol	Chain	Res	Type
1	A	329	PRO

5.3.2 Protein sidechains

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	275/375 (73%)	230 (84%)	45 (16%)	3 8

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	64	PRO
1	A	71	TYR
1	A	78	ARG
1	A	82	SER
1	A	102	ASP
1	A	126	ARG
1	A	149	VAL
1	A	154	ASN
1	A	155	PHE
1	A	161	CYS
1	A	169	LEU
1	A	175	LEU
1	A	179	GLN
1	A	180	PHE
1	A	182	ASP
1	A	203	PHE
1	A	215	TYR
1	A	236	THR
1	A	238	LEU
1	A	242	ILE
1	A	250	GLU
1	A	255	GLN
1	A	272	ASN
1	A	274	SER

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Mol	Chain	Res	Type
1	A	275	ARG
1	A	287	ASP
1	A	298	ASP
1	A	304	ASP
1	A	317	GLU
1	A	319	THR
1	A	321	PRO
1	A	342	ASP
1	A	347	MET
1	A	348	ASP
1	A	384	TRP
1	A	392	PRO
1	A	393	ASN
1	A	404	PRO
1	A	412	LEU
1	A	414	PRO
1	A	423	ILE
1	A	428	TRP
1	A	449	ASP
1	A	458	LEU

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

Mol	Chain	Res	Type
1	A	130	HIS
1	A	137	ASN
1	A	207	HIS
1	A	255	GLN
1	A	355	GLN
1	A	371	GLN
1	A	393	ASN
1	A	395	GLN
1	A	405	ASN
1	A	438	ASN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	380/424 (89%)	0.51	27 (7%) 19 13	23, 59, 89, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	PRO	5.5
1	A	63	ALA	5.3
1	A	458	LEU	3.7
1	A	130	HIS	3.6
1	A	341	GLU	3.6
1	A	287	ASP	3.3
1	A	272	ASN	3.1
1	A	65	VAL	3.0
1	A	448	VAL	2.8
1	A	404	PRO	2.8
1	A	196	GLY	2.8
1	A	127	ALA	2.8
1	A	301	LYS	2.7
1	A	215	TYR	2.6
1	A	281	GLU	2.6
1	A	430	MET	2.5
1	A	274	SER	2.5
1	A	115	LEU	2.4
1	A	442	CYS	2.2
1	A	260	SER	2.2
1	A	133	SER	2.1
1	A	114	LYS	2.1
1	A	405	ASN	2.1
1	A	444	ASP	2.1
1	A	398	TRP	2.1
1	A	125	SER	2.0
1	A	337	ALA	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 (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
2	CA	A	900	1/1	0.83	0.11	-2.97	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.