



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:08 pm GMT

PDB ID : 3NC1
Title : Crystal structure of the CRM1-RanGTP complex
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Deposited on : 2010-06-04
Resolution : 3.35 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

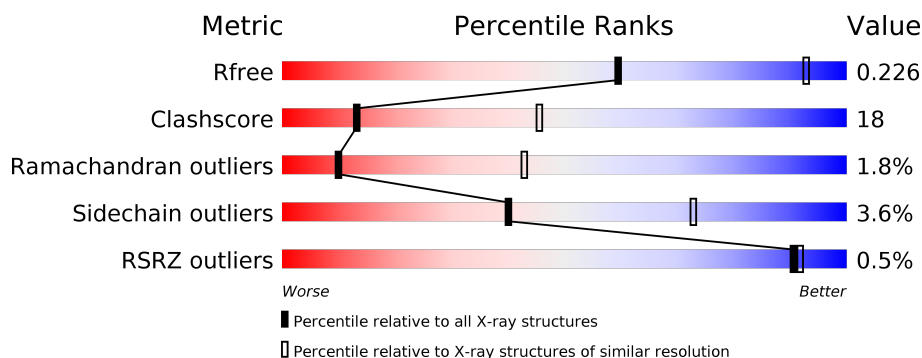
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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	C	182	<div> <div></div> <div>60%</div> <div>30%</div> <div>5%</div> <div>5%</div> </div>
2	A	1073	<div> <div>57%</div> <div>36%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9749 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	173	Total	C	N	O	S	0	0	0
			1403	912	246	241	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P62826
C	0	SER	-	expression tag	UNP P62826
C	69	LEU	GLN	engineered	UNP P62826

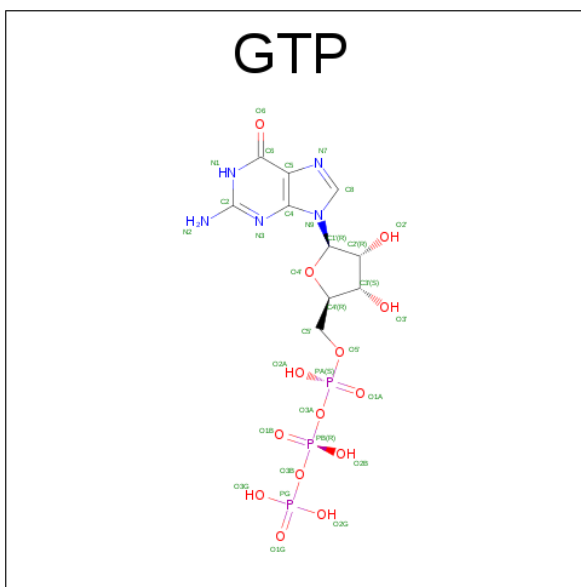
- Molecule 2 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1026	Total	C	N	O	S	0	0	0
			8313	5335	1394	1531	53			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

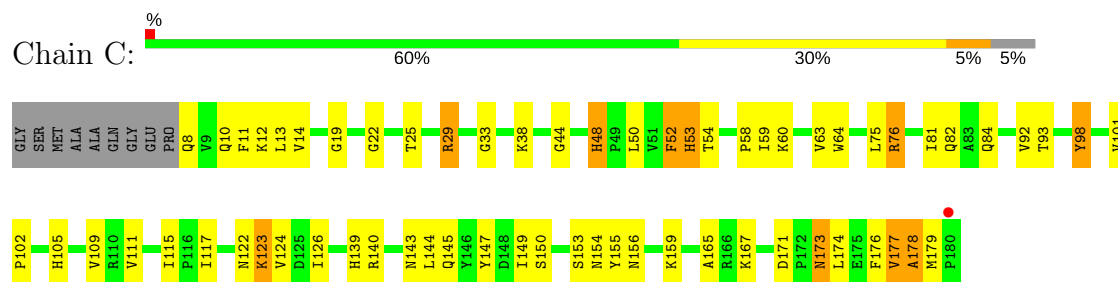
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

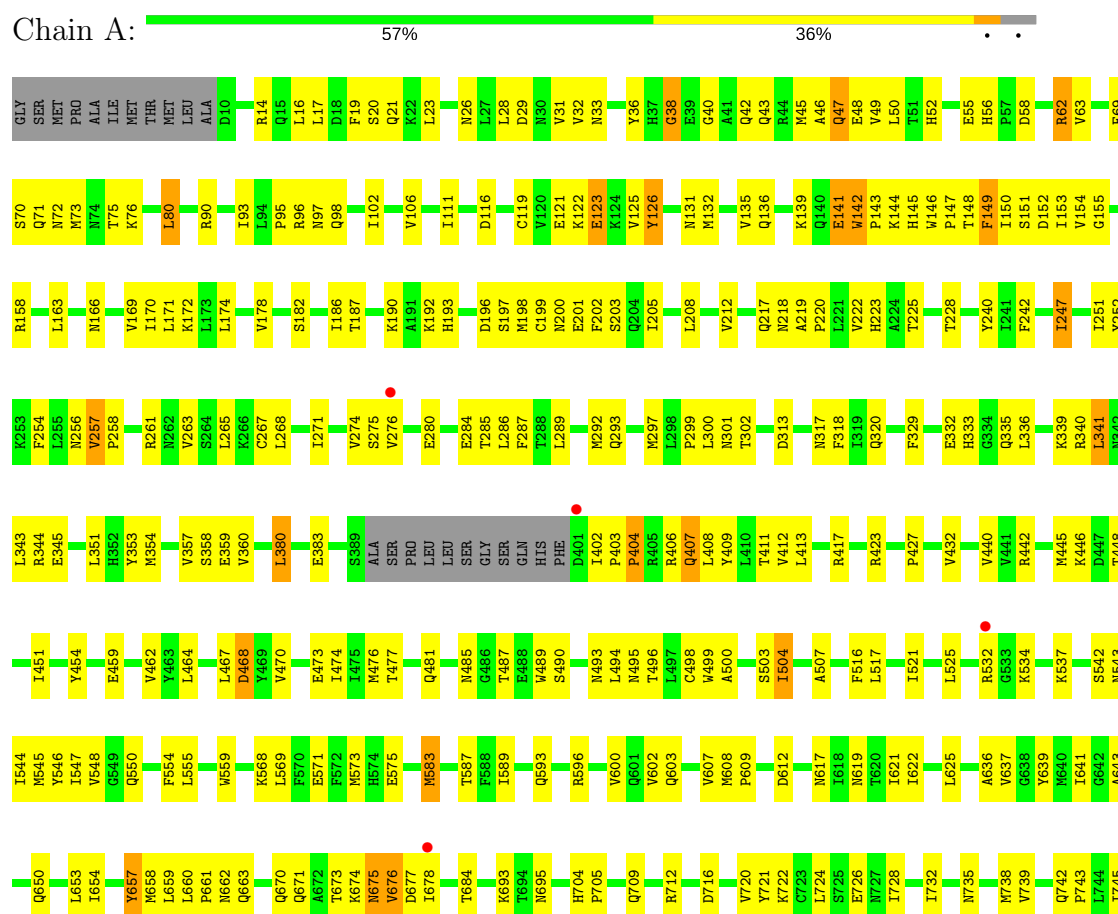
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GTP-binding nuclear protein Ran



• Molecule 2: Exportin-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.80Å 216.16Å 123.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.52 – 3.35 36.52 – 3.35	Depositor EDS
% Data completeness (in resolution range)	86.5 (36.52-3.35) 86.7 (36.52-3.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.219 , 0.254 0.209 , 0.226	Depositor DCC
R_{free} test set	1322 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	114.8	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9749	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.22	0/1438	0.38	0/1942
2	A	0.21	0/8481	0.37	0/11486
All	All	0.21	0/9919	0.37	0/13428

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	C	1403	0	1426	52	0
2	A	8313	0	8369	310	0
3	C	32	0	12	7	0
4	C	1	0	0	0	0
All	All	9749	0	9807	355	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 18.

All (355) 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)
2:A:28:LEU:HD21	2:A:70:SER:HB2	1.48	0.94
2:A:1004:LEU:HD23	2:A:1004:LEU:H	1.40	0.86
2:A:602:VAL:HG22	2:A:609:PRO:HD3	1.56	0.85
1:C:53:HIS:HA	1:C:58:PRO:HA	1.56	0.84
1:C:8:GLN:HG3	1:C:58:PRO:HG2	1.58	0.83
2:A:351:LEU:HD23	2:A:412:VAL:HG21	1.62	0.80
2:A:432:VAL:HG22	2:A:442:ARG:HG2	1.64	0.79
2:A:1008:ILE:HG13	2:A:1009:PRO:HD3	1.66	0.78
2:A:256:ASN:HB3	2:A:293:GLN:HE21	1.49	0.78
2:A:532:ARG:HA	2:A:537:LYS:HE3	1.66	0.77
2:A:545:MET:HB3	2:A:587:THR:HG21	1.65	0.77
2:A:675:ASN:HD21	2:A:677:ASP:HB2	1.50	0.77
2:A:756:LEU:HD22	2:A:803:THR:HG21	1.67	0.77
1:C:81:ILE:HG22	1:C:82:GLN:HG3	1.64	0.77
2:A:952:LEU:HD23	2:A:956:GLY:HA3	1.68	0.76
1:C:22:GLY:HA2	3:C:181:GTP:H5''	1.66	0.76
2:A:172:LYS:HB2	2:A:228:THR:HB	1.69	0.74
2:A:69:PHE:HB2	2:A:76:LYS:HE2	1.69	0.74
2:A:339:LYS:HG3	2:A:340:ARG:H	1.53	0.74
2:A:17:LEU:HD12	2:A:23:LEU:HD11	1.70	0.73
2:A:242:PHE:HA	2:A:247:ILE:HD11	1.71	0.72
2:A:219:ALA:HB3	2:A:220:PRO:HD3	1.72	0.71
2:A:417:ARG:HH12	2:A:468:ASP:HB3	1.56	0.71
2:A:498:CYS:SG	2:A:543:ASN:HB3	2.31	0.71
2:A:969:ASN:ND2	2:A:972:MET:H	1.89	0.70
2:A:496:THR:HA	2:A:499:TRP:CE3	2.25	0.70
2:A:969:ASN:HD22	2:A:972:MET:H	1.41	0.69
2:A:146:TRP:N	2:A:147:PRO:HD3	2.07	0.69
2:A:963:ASN:HB2	2:A:964:PRO:HD3	1.74	0.68
1:C:53:HIS:ND1	1:C:58:PRO:HB3	2.09	0.67
1:C:38:LYS:HB3	2:A:842:PRO:HG3	1.77	0.67
2:A:819:ILE:HD13	2:A:822:ILE:HD12	1.76	0.66
1:C:139:HIS:HB2	1:C:144:LEU:HB2	1.78	0.66
2:A:408:LEU:HD22	2:A:408:LEU:H	1.60	0.66
1:C:25:THR:OG1	3:C:181:GTP:H5'	1.96	0.65
2:A:548:VAL:HG13	2:A:555:LEU:HD21	1.78	0.65
2:A:402:ILE:HG21	2:A:407:GLN:HE22	1.61	0.65
2:A:805:ALA:HB2	2:A:851:LEU:HA	1.77	0.65
2:A:653:LEU:O	2:A:657:TYR:HB2	1.97	0.65
2:A:607:VAL:HG23	2:A:608:MET:H	1.62	0.64
2:A:111:ILE:HG23	2:A:163:LEU:HD21	1.80	0.64
2:A:760:SER:HB3	2:A:803:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:ARG:HH11	2:A:45:MET:HG3	1.64	0.63
2:A:131:ASN:HD22	2:A:170:ILE:HD11	1.63	0.63
2:A:62:ARG:NH1	2:A:63:VAL:HA	2.14	0.63
2:A:957:LYS:NZ	2:A:961:PRO:HG3	2.15	0.61
2:A:788:TYR:CE1	2:A:796:ARG:HB3	2.35	0.61
2:A:1038:ARG:O	2:A:1042:LEU:HG	2.00	0.61
2:A:33:ASN:OD1	2:A:42:GLN:HB3	2.00	0.61
2:A:798:PRO:HB2	2:A:847:ASN:HD22	1.66	0.61
1:C:177:VAL:O	1:C:178:ALA:HB3	2.01	0.61
2:A:801:LEU:HB2	2:A:847:ASN:HB3	1.82	0.60
2:A:403:PRO:HB2	2:A:406:ARG:HB2	1.83	0.60
1:C:12:LYS:HE3	1:C:64:TRP:CE2	2.37	0.60
2:A:353:TYR:O	2:A:357:VAL:HG12	2.02	0.59
2:A:285:THR:O	2:A:289:LEU:HB2	2.02	0.59
2:A:796:ARG:O	2:A:844:HIS:HE1	1.85	0.59
2:A:151:SER:HA	2:A:154:VAL:HG12	1.84	0.59
1:C:156:ASN:ND2	1:C:159:LYS:HD2	2.18	0.59
2:A:670:GLN:HE21	2:A:674:LYS:HE2	1.66	0.59
1:C:153:SER:O	1:C:154:ASN:HB2	2.03	0.59
2:A:695:ASN:HD21	2:A:709:GLN:HE21	1.50	0.59
2:A:957:LYS:HZ1	2:A:961:PRO:HG3	1.68	0.59
1:C:117:ILE:HB	1:C:144:LEU:HD22	1.84	0.59
2:A:383:GLU:OE2	2:A:404:PRO:HG2	2.03	0.59
2:A:569:LEU:O	2:A:573:MET:HG2	2.03	0.59
2:A:704:HIS:HD2	2:A:767:ASN:H	1.49	0.58
2:A:785:LEU:HD22	2:A:826:VAL:HG11	1.85	0.58
2:A:276:VAL:HB	2:A:333:HIS:CE1	2.39	0.58
2:A:142:TRP:HB3	2:A:143:PRO:HD3	1.85	0.58
1:C:147:TYR:CE1	1:C:159:LYS:HD3	2.39	0.58
2:A:1040:THR:HG22	2:A:1043:ARG:HH21	1.69	0.57
2:A:467:LEU:O	2:A:468:ASP:HB2	2.04	0.57
2:A:908:GLU:HA	2:A:911:ALA:HB3	1.86	0.57
2:A:609:PRO:HG2	2:A:612:ASP:OD1	2.04	0.57
2:A:170:ILE:HG22	2:A:171:LEU:HD23	1.87	0.57
2:A:542:SER:HA	2:A:583:MET:SD	2.45	0.57
2:A:354:MET:O	2:A:358:SER:HB2	2.05	0.57
2:A:753:ARG:HG3	2:A:799:GLU:HG3	1.85	0.57
1:C:124:VAL:HG22	1:C:150:SER:HB2	1.86	0.56
1:C:123:LYS:HE2	3:C:181:GTP:N9	2.21	0.56
2:A:43:GLN:HA	2:A:46:ALA:HB3	1.86	0.56
2:A:495:ASN:HA	2:A:543:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HD2	1:C:76:ARG:H	1.71	0.56
2:A:251:ILE:HD11	2:A:286:LEU:HD12	1.88	0.56
2:A:359:GLU:HA	2:A:423:ARG:NH1	2.21	0.56
2:A:417:ARG:NH1	2:A:468:ASP:HB3	2.19	0.55
1:C:123:LYS:HE2	3:C:181:GTP:C8	2.41	0.55
2:A:149:PHE:CZ	2:A:153:ILE:HD11	2.40	0.55
2:A:658:MET:HE2	2:A:661:PRO:HG2	1.88	0.55
2:A:543:ASN:O	2:A:547:ILE:HG12	2.06	0.55
1:C:10:GLN:HB3	1:C:60:LYS:HB3	1.87	0.55
2:A:1040:THR:O	2:A:1044:GLN:HB2	2.06	0.55
2:A:186:ILE:HD11	2:A:190:LYS:HE3	1.89	0.55
2:A:19:PHE:HD1	2:A:56:HIS:HE1	1.54	0.55
2:A:252:TYR:CE2	2:A:289:LEU:HD21	2.42	0.54
2:A:675:ASN:ND2	2:A:677:ASP:HB2	2.19	0.54
2:A:739:VAL:O	2:A:742:GLN:HG2	2.07	0.54
2:A:149:PHE:O	2:A:153:ILE:HG13	2.07	0.54
2:A:427:PRO:HG3	2:A:546:TYR:OH	2.07	0.54
2:A:670:GLN:O	2:A:673:THR:HG22	2.07	0.54
2:A:950:PHE:CE1	2:A:1001:LEU:HB3	2.43	0.54
2:A:218:ASN:OD1	2:A:220:PRO:HD2	2.08	0.54
2:A:299:PRO:HB2	2:A:302:THR:HG23	1.90	0.54
2:A:872:LYS:O	2:A:876:ASP:HB2	2.08	0.54
2:A:339:LYS:HG3	2:A:340:ARG:N	2.22	0.53
2:A:786:ILE:O	2:A:790:ARG:HG3	2.09	0.53
1:C:11:PHE:HD1	1:C:84:GLN:HG2	1.74	0.53
2:A:559:TRP:CE2	2:A:603:GLN:HG3	2.43	0.53
2:A:32:VAL:O	2:A:36:TYR:HB2	2.07	0.53
2:A:622:ILE:HG22	2:A:625:LEU:HD12	1.90	0.53
2:A:593:GLN:HG2	2:A:639:TYR:CD2	2.43	0.53
2:A:939:LEU:C	2:A:939:LEU:HD23	2.29	0.53
2:A:837:ASP:OD2	2:A:840:GLU:HG2	2.08	0.53
2:A:14:ARG:NH1	2:A:45:MET:HG3	2.23	0.53
2:A:517:LEU:HD12	2:A:554:PHE:CD1	2.43	0.53
2:A:728:ILE:HD12	2:A:752:LYS:HD3	1.91	0.53
2:A:193:HIS:O	2:A:197:SER:HB2	2.09	0.53
2:A:202:PHE:HD1	2:A:205:ILE:HD11	1.74	0.53
2:A:280:GLU:HG3	2:A:336:LEU:HD13	1.92	0.52
2:A:704:HIS:CD2	2:A:767:ASN:H	2.26	0.52
2:A:659:LEU:O	2:A:663:GLN:HG3	2.09	0.52
1:C:11:PHE:CE2	1:C:59:ILE:HD11	2.44	0.52
2:A:16:LEU:HD12	2:A:49:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:PHE:HB2	2:A:329:PHE:CZ	2.45	0.52
2:A:818:GLU:O	2:A:822:ILE:HG13	2.10	0.52
2:A:29:ASP:O	2:A:33:ASN:HB2	2.10	0.52
1:C:98:TYR:CD2	1:C:98:TYR:C	2.83	0.52
1:C:92:VAL:HG22	1:C:122:ASN:O	2.09	0.52
2:A:1004:LEU:HD11	2:A:1014:HIS:HB2	1.93	0.51
2:A:28:LEU:HD12	2:A:75:THR:HG21	1.93	0.51
2:A:417:ARG:HD3	2:A:464:LEU:O	2.11	0.51
2:A:427:PRO:HB3	2:A:454:TYR:CE1	2.46	0.51
2:A:840:GLU:O	2:A:845:ARG:NH1	2.44	0.51
1:C:167:LYS:HE2	2:A:313:ASP:OD2	2.11	0.51
2:A:800:VAL:HA	2:A:803:THR:HG22	1.93	0.51
2:A:476:MET:HG2	2:A:516:PHE:HZ	1.77	0.50
2:A:716:ASP:O	2:A:720:VAL:HG12	2.10	0.50
2:A:879:ILE:HA	2:A:882:PHE:CE2	2.46	0.50
1:C:105:HIS:CE1	1:C:109:VAL:HG11	2.46	0.50
2:A:500:ALA:O	2:A:503:SER:HB3	2.12	0.50
2:A:90:ARG:HB2	2:A:93:ILE:HD11	1.93	0.50
1:C:177:VAL:O	1:C:178:ALA:CB	2.59	0.50
1:C:19:GLY:HA2	3:C:181:GTP:O3G	2.12	0.50
2:A:781:LEU:HD11	2:A:821:GLN:OE1	2.12	0.50
1:C:115:ILE:O	1:C:117:ILE:HG13	2.12	0.50
2:A:76:LYS:O	2:A:80:LEU:HD13	2.12	0.49
2:A:268:LEU:HD22	2:A:286:LEU:HD11	1.94	0.49
2:A:949:MET:O	2:A:953:VAL:HG23	2.11	0.49
1:C:149:ILE:HA	1:C:155:TYR:O	2.12	0.49
2:A:1044:GLN:O	2:A:1048:GLU:HG2	2.12	0.49
1:C:123:LYS:HG3	3:C:181:GTP:C5	2.48	0.49
2:A:596:ARG:HD3	2:A:643:ALA:HB2	1.93	0.49
2:A:261:ARG:HG2	2:A:318:PHE:CE1	2.47	0.49
2:A:459:GLU:O	2:A:462:VAL:HG12	2.13	0.49
2:A:489:TRP:HZ3	2:A:494:LEU:HD22	1.77	0.49
2:A:912:GLN:CD	2:A:958:ILE:HG12	2.32	0.49
2:A:261:ARG:HG2	2:A:318:PHE:CD1	2.47	0.49
2:A:19:PHE:HD1	2:A:56:HIS:CE1	2.31	0.49
1:C:13:LEU:HD23	1:C:14:VAL:N	2.28	0.49
2:A:252:TYR:OH	2:A:289:LEU:HD11	2.13	0.49
2:A:495:ASN:HA	2:A:543:ASN:ND2	2.27	0.49
2:A:608:MET:HB3	2:A:609:PRO:HD2	1.95	0.49
2:A:71:GLN:O	2:A:71:GLN:HG2	2.13	0.49
2:A:446:LYS:O	2:A:451:ILE:HG21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:548:VAL:HG12	2:A:555:LEU:HD11	1.94	0.48
2:A:172:LYS:HB2	2:A:228:THR:CB	2.39	0.48
2:A:131:ASN:O	2:A:135:VAL:HG23	2.12	0.48
2:A:20:SER:O	2:A:21:GLN:HG3	2.13	0.48
1:C:38:LYS:HB3	2:A:842:PRO:CG	2.42	0.48
2:A:660:LEU:HB2	2:A:661:PRO:HD3	1.96	0.48
2:A:69:PHE:HD1	2:A:71:GLN:H	1.60	0.48
2:A:778:PRO:HB2	2:A:779:PRO:HD3	1.96	0.48
1:C:122:ASN:O	1:C:123:LYS:HB2	2.14	0.48
2:A:721:TYR:CE1	2:A:752:LYS:HG2	2.49	0.48
2:A:743:PRO:O	2:A:746:ARG:HB2	2.14	0.48
2:A:745:ILE:O	2:A:745:ILE:HG22	2.14	0.48
2:A:872:LYS:HD3	2:A:872:LYS:O	2.13	0.48
2:A:477:THR:O	2:A:481:GLN:HG2	2.13	0.47
2:A:265:LEU:HD22	2:A:318:PHE:CE1	2.49	0.47
2:A:73:MET:HG3	2:A:123:GLU:HG3	1.95	0.47
2:A:402:ILE:CG2	2:A:407:GLN:HE22	2.26	0.47
2:A:485:ASN:C	2:A:487:THR:H	2.18	0.47
2:A:860:PHE:N	2:A:861:PRO:CD	2.78	0.47
1:C:48:HIS:N	1:C:48:HIS:CD2	2.83	0.47
2:A:150:ILE:HD12	2:A:201:GLU:HG3	1.97	0.47
2:A:256:ASN:HA	2:A:297:MET:SD	2.55	0.47
2:A:838:PHE:HD1	2:A:884:HIS:CD2	2.32	0.47
1:C:111:VAL:HA	2:A:125:VAL:HG13	1.97	0.47
2:A:759:ILE:O	2:A:763:VAL:HG23	2.14	0.47
2:A:172:LYS:HD2	2:A:228:THR:HG22	1.97	0.46
2:A:589:ILE:O	2:A:593:GLN:HG3	2.15	0.46
1:C:53:HIS:CD2	1:C:53:HIS:N	2.84	0.46
1:C:29:ARG:O	1:C:33:GLY:HA2	2.13	0.46
2:A:119:CYS:HA	2:A:122:LYS:HD3	1.96	0.46
2:A:568:LYS:O	2:A:571:GLU:HB3	2.15	0.46
2:A:637:VAL:O	2:A:641:ILE:HG12	2.15	0.46
2:A:671:GLN:HG2	2:A:678:ILE:HG12	1.96	0.46
2:A:1013:GLU:O	2:A:1017:ASP:HB2	2.16	0.46
2:A:409:TYR:O	2:A:413:LEU:HG	2.16	0.46
2:A:487:THR:C	2:A:489:TRP:H	2.19	0.46
1:C:123:LYS:HG3	3:C:181:GTP:C6	2.51	0.46
2:A:132:MET:CE	2:A:132:MET:HA	2.45	0.46
2:A:252:TYR:CZ	2:A:289:LEU:HD21	2.51	0.46
2:A:98:GLN:O	2:A:102:ILE:HG13	2.16	0.46
2:A:950:PHE:CD1	2:A:1001:LEU:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:153:ILE:C	2:A:155:GLY:H	2.18	0.46
2:A:650:GLN:O	2:A:654:ILE:HG13	2.15	0.46
2:A:772:VAL:HB	2:A:811:LEU:HD21	1.97	0.46
2:A:196:ASP:HA	2:A:199:CYS:HB3	1.97	0.46
2:A:178:VAL:HB	2:A:198:MET:HE1	1.97	0.46
2:A:31:VAL:HG21	2:A:75:THR:HG23	1.97	0.46
2:A:792:VAL:HG23	2:A:793:PRO:HD2	1.97	0.46
2:A:202:PHE:CD1	2:A:205:ILE:HD11	2.50	0.46
2:A:1016:ARG:O	2:A:1020:VAL:HG23	2.16	0.45
2:A:32:VAL:HG12	2:A:32:VAL:O	2.15	0.45
2:A:96:ARG:HD3	2:A:96:ARG:HA	1.78	0.45
1:C:8:GLN:CG	1:C:58:PRO:HG2	2.38	0.45
2:A:489:TRP:CZ3	2:A:494:LEU:HD22	2.51	0.45
2:A:102:ILE:O	2:A:106:VAL:HG23	2.17	0.45
2:A:187:THR:OG1	2:A:190:LYS:HB3	2.15	0.45
2:A:344:ARG:HD3	2:A:408:LEU:HD12	1.98	0.45
2:A:132:MET:HE2	2:A:132:MET:HA	1.98	0.45
2:A:148:THR:O	2:A:149:PHE:C	2.54	0.45
2:A:28:LEU:HD11	2:A:70:SER:OG	2.16	0.45
1:C:93:THR:HG21	1:C:126:ILE:HD12	1.99	0.45
2:A:132:MET:O	2:A:136:GLN:HG2	2.16	0.45
2:A:178:VAL:O	2:A:182:SER:HB3	2.15	0.45
1:C:155:TYR:CE1	2:A:445:MET:HG3	2.51	0.45
2:A:1003:SER:HA	2:A:1046:GLN:OE1	2.16	0.45
2:A:742:GLN:HB2	2:A:743:PRO:HD2	1.99	0.45
2:A:875:LEU:HD13	2:A:875:LEU:O	2.16	0.45
2:A:126:TYR:C	2:A:126:TYR:CD2	2.90	0.45
2:A:777:VAL:HB	2:A:778:PRO:HD3	1.98	0.45
2:A:589:ILE:HG13	2:A:636:ALA:HA	1.98	0.45
2:A:738:MET:CE	2:A:738:MET:HA	2.47	0.45
2:A:254:PHE:O	2:A:257:VAL:HG13	2.16	0.45
2:A:146:TRP:N	2:A:147:PRO:CD	2.80	0.44
2:A:658:MET:HE2	2:A:658:MET:HA	1.99	0.44
2:A:292:MET:HG3	2:A:293:GLN:N	2.32	0.44
2:A:174:LEU:HD22	2:A:198:MET:SD	2.58	0.44
2:A:300:LEU:HD12	2:A:300:LEU:N	2.33	0.44
2:A:802:SER:C	2:A:804:MET:H	2.20	0.44
1:C:75:LEU:O	1:C:76:ARG:C	2.55	0.44
2:A:473:GLU:HG3	2:A:516:PHE:CD1	2.53	0.44
2:A:490:SER:HB3	2:A:493:ASN:CG	2.38	0.44
2:A:521:ILE:O	2:A:525:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:223:HIS:CE1	2:A:263:VAL:HG21	2.53	0.44
1:C:98:TYR:C	1:C:98:TYR:HD2	2.20	0.44
2:A:47:GLN:HG3	2:A:48:GLU:N	2.33	0.44
1:C:145:GLN:HA	1:C:145:GLN:HE21	1.83	0.44
2:A:276:VAL:O	2:A:276:VAL:HG22	2.18	0.43
2:A:448:THR:OG1	2:A:451:ILE:HG22	2.18	0.43
2:A:704:HIS:HB3	2:A:705:PRO:HD3	1.99	0.43
2:A:929:VAL:HG13	2:A:935:HIS:CG	2.52	0.43
1:C:165:ALA:HB1	1:C:174:LEU:HD23	1.99	0.43
2:A:276:VAL:HB	2:A:333:HIS:ND1	2.33	0.43
2:A:141:GLU:HG3	2:A:145:HIS:HD2	1.82	0.43
2:A:38:GLY:HA2	2:A:42:GLN:HB2	1.99	0.43
2:A:380:LEU:HD12	2:A:380:LEU:HA	1.81	0.43
2:A:781:LEU:O	2:A:786:ILE:HG13	2.18	0.43
2:A:892:THR:O	2:A:896:ILE:HG13	2.18	0.43
2:A:257:VAL:HA	2:A:258:PRO:HD3	1.92	0.43
2:A:504:ILE:O	2:A:504:ILE:HD12	2.18	0.43
2:A:617:ASN:O	2:A:621:ILE:HG13	2.19	0.43
2:A:841:TYR:N	2:A:842:PRO:HD3	2.34	0.43
2:A:954:GLU:O	2:A:955:GLU:HG3	2.19	0.43
2:A:212:VAL:HB	2:A:225:THR:HG21	2.00	0.43
1:C:143:ASN:HA	2:A:320:GLN:HE22	1.84	0.43
2:A:332:GLU:HG3	2:A:332:GLU:O	2.19	0.43
2:A:341:LEU:HG	2:A:344:ARG:HH21	1.84	0.43
2:A:517:LEU:HD12	2:A:554:PHE:CG	2.53	0.43
2:A:735:ASN:HB3	2:A:739:VAL:HG11	2.00	0.43
2:A:759:ILE:HD13	2:A:780:LEU:HD21	2.01	0.43
2:A:816:THR:HG23	2:A:862:ALA:HB2	2.01	0.43
2:A:123:GLU:OE1	2:A:125:VAL:HB	2.19	0.43
2:A:166:ASN:O	2:A:169:VAL:HG12	2.19	0.43
2:A:274:VAL:HG12	2:A:275:SER:N	2.33	0.43
2:A:299:PRO:C	2:A:301:ASN:H	2.22	0.43
2:A:148:THR:HB	2:A:152:ASP:OD1	2.19	0.42
1:C:101:VAL:N	1:C:102:PRO:CD	2.82	0.42
2:A:335:GLN:O	2:A:339:LYS:HG2	2.18	0.42
2:A:837:ASP:O	2:A:880:TRP:HZ2	2.02	0.42
2:A:897:LEU:O	2:A:901:LEU:HG	2.19	0.42
2:A:956:GLY:O	2:A:958:ILE:HG23	2.19	0.42
1:C:171:ASP:C	1:C:173:ASN:H	2.23	0.42
1:C:54:THR:HG22	1:C:176:PHE:CD1	2.53	0.42
2:A:545:MET:CE	2:A:545:MET:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:918:TYR:O	2:A:919:PHE:C	2.58	0.42
2:A:116:ASP:HB3	2:A:119:CYS:SG	2.59	0.42
2:A:126:TYR:C	2:A:126:TYR:HD2	2.22	0.42
2:A:192:LYS:HE3	2:A:196:ASP:OD1	2.19	0.42
2:A:208:LEU:HD23	2:A:208:LEU:O	2.19	0.42
2:A:284:GLU:HG3	2:A:343:LEU:HD21	2.00	0.42
2:A:728:ILE:O	2:A:732:ILE:HG12	2.18	0.42
2:A:875:LEU:O	2:A:879:ILE:HG12	2.20	0.42
2:A:95:PRO:HB2	2:A:97:ASN:ND2	2.34	0.42
2:A:1021:GLN:HE21	2:A:1033:LEU:HD13	1.84	0.42
2:A:544:ILE:O	2:A:548:VAL:HG23	2.20	0.42
2:A:948:TYR:O	2:A:952:LEU:HB2	2.20	0.42
2:A:950:PHE:HE1	2:A:1001:LEU:HD13	1.82	0.42
2:A:203:SER:HB3	2:A:240:TYR:OH	2.20	0.42
2:A:256:ASN:HB3	2:A:293:GLN:NE2	2.26	0.42
2:A:676:VAL:HG12	2:A:676:VAL:O	2.20	0.42
2:A:73:MET:HG3	2:A:123:GLU:CG	2.50	0.42
2:A:860:PHE:HE1	2:A:900:LEU:HD22	1.85	0.42
2:A:926:ILE:O	2:A:930:VAL:HG23	2.20	0.42
2:A:339:LYS:HE3	2:A:339:LYS:HB2	1.87	0.42
2:A:722:LYS:O	2:A:726:GLU:HG3	2.19	0.42
2:A:693:LYS:HB2	2:A:693:LYS:HE3	1.89	0.41
2:A:351:LEU:HD21	2:A:409:TYR:HD1	1.84	0.41
2:A:662:ASN:HD22	2:A:712:ARG:CZ	2.34	0.41
2:A:887:ARG:NH1	2:A:887:ARG:HB2	2.35	0.41
2:A:121:GLU:O	2:A:121:GLU:HG2	2.20	0.41
2:A:951:ASN:HD22	2:A:1005:ASN:HD21	1.69	0.41
2:A:1008:ILE:CG1	2:A:1009:PRO:HD3	2.44	0.41
2:A:182:SER:O	2:A:186:ILE:HG22	2.19	0.41
2:A:247:ILE:HG13	2:A:247:ILE:H	1.53	0.41
2:A:267:CYS:O	2:A:271:ILE:HG13	2.20	0.41
2:A:546:TYR:O	2:A:550:GLN:HG2	2.20	0.41
2:A:46:ALA:O	2:A:50:LEU:HG	2.21	0.41
2:A:724:LEU:HD22	2:A:748:MET:HE2	2.02	0.41
2:A:838:PHE:HA	2:A:845:ARG:HH21	1.85	0.41
2:A:989:LEU:HA	2:A:993:GLN:HE21	1.85	0.41
2:A:222:VAL:HG11	2:A:254:PHE:HE1	1.85	0.41
2:A:357:VAL:O	2:A:360:VAL:HG23	2.20	0.41
2:A:534:LYS:HE3	2:A:575:GLU:OE2	2.21	0.41
2:A:600:VAL:O	2:A:609:PRO:HB3	2.21	0.41
2:A:867:PRO:HA	2:A:868:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:VAL:O	2:A:158:ARG:HD2	2.20	0.41
2:A:131:ASN:ND2	2:A:170:ILE:HD11	2.31	0.41
2:A:470:VAL:O	2:A:474:ILE:HD13	2.20	0.41
2:A:494:LEU:HG	2:A:543:ASN:HD22	1.86	0.41
2:A:793:PRO:HA	2:A:796:ARG:HD2	2.02	0.41
2:A:798:PRO:HB2	2:A:847:ASN:ND2	2.32	0.41
2:A:837:ASP:O	2:A:845:ARG:NH2	2.53	0.41
2:A:904:VAL:HG13	2:A:911:ALA:HA	2.02	0.41
2:A:952:LEU:O	2:A:952:LEU:HD23	2.20	0.41
2:A:997:PHE:CE2	2:A:1001:LEU:HD11	2.56	0.41
2:A:1004:LEU:CD2	2:A:1004:LEU:H	2.20	0.41
2:A:1008:ILE:N	2:A:1009:PRO:CD	2.83	0.41
2:A:14:ARG:HA	2:A:14:ARG:HD2	1.89	0.41
2:A:568:LYS:HD2	2:A:568:LYS:HA	1.90	0.41
2:A:724:LEU:O	2:A:728:ILE:HG13	2.20	0.41
2:A:1048:GLU:C	2:A:1050:HIS:H	2.24	0.41
2:A:143:PRO:HG2	2:A:193:HIS:CE1	2.55	0.41
2:A:607:VAL:HG23	2:A:608:MET:N	2.32	0.41
2:A:704:HIS:N	2:A:705:PRO:CD	2.84	0.40
1:C:52:PHE:O	1:C:59:ILE:HG22	2.20	0.40
2:A:135:VAL:O	2:A:139:LYS:HG3	2.20	0.40
2:A:462:VAL:HG23	2:A:507:ALA:HB2	2.03	0.40
2:A:251:ILE:HD11	2:A:286:LEU:CD1	2.51	0.40
1:C:50:LEU:HD12	1:C:63:VAL:HG21	2.03	0.40
2:A:923:LEU:O	2:A:927:PHE:HD1	2.04	0.40
1:C:143:ASN:HB3	2:A:317:ASN:ND2	2.37	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	C	171/182 (94%)	144 (84%)	22 (13%)	5 (3%)	5	33
2	A	1020/1073 (95%)	895 (88%)	109 (11%)	16 (2%)	11	45
All	All	1191/1255 (95%)	1039 (87%)	131 (11%)	21 (2%)	10	43

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	76	ARG
2	A	149	PHE
2	A	468	ASP
1	C	44	GLY
1	C	178	ALA
2	A	144	LYS
2	A	956	GLY
2	A	58	ASP
2	A	142	TRP
2	A	404	PRO
2	A	504	ILE
2	A	675	ASN
2	A	676	VAL
2	A	837	ASP
1	C	179	MET
2	A	38	GLY
2	A	657	TYR
1	C	140	ARG
2	A	123	GLU
2	A	886	MET
2	A	40	GLY

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	C	151/157 (96%)	143 (95%)	8 (5%)	26	63
2	A	933/973 (96%)	902 (97%)	31 (3%)	43	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1084/1130 (96%)	1045 (96%)	39 (4%)	40 73

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	ARG
1	C	48	HIS
1	C	52	PHE
1	C	53	HIS
1	C	98	TYR
1	C	123	LYS
1	C	173	ASN
1	C	177	VAL
2	A	26	ASN
2	A	47	GLN
2	A	52	HIS
2	A	55	GLU
2	A	62	ARG
2	A	72	ASN
2	A	80	LEU
2	A	126	TYR
2	A	141	GLU
2	A	200	ASN
2	A	217	GLN
2	A	247	ILE
2	A	257	VAL
2	A	341	LEU
2	A	345	GLU
2	A	380	LEU
2	A	407	GLN
2	A	411	THR
2	A	440	VAL
2	A	583	MET
2	A	619	ASN
2	A	684	THR
2	A	792	VAL
2	A	807	ILE
2	A	876	ASP
2	A	885	THR
2	A	898	PHE
2	A	927	PHE
2	A	960	THR

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Mol	Chain	Res	Type
2	A	1004	LEU
2	A	1011	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	HIS
1	C	82	GLN
1	C	105	HIS
1	C	145	GLN
1	C	156	ASN
1	C	173	ASN
2	A	26	ASN
2	A	56	HIS
2	A	97	ASN
2	A	131	ASN
2	A	145	HIS
2	A	165	GLN
2	A	166	ASN
2	A	217	GLN
2	A	223	HIS
2	A	293	GLN
2	A	317	ASN
2	A	320	GLN
2	A	321	ASN
2	A	407	GLN
2	A	466	HIS
2	A	543	ASN
2	A	550	GLN
2	A	558	HIS
2	A	577	HIS
2	A	593	GLN
2	A	601	GLN
2	A	619	ASN
2	A	626	GLN
2	A	670	GLN
2	A	675	ASN
2	A	695	ASN
2	A	704	HIS
2	A	844	HIS
2	A	847	ASN
2	A	853	GLN

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Mol	Chain	Res	Type
2	A	870	GLN
2	A	916	GLN
2	A	951	ASN
2	A	969	ASN
2	A	975	GLN
2	A	980	ASN
2	A	993	GLN
2	A	1021	GLN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GTP	C	181	4	27,34,34	0.94	1 (3%)	27,54,54	1.73	5 (18%)

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	GTP	C	181	4	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	GTP	C6-N1	3.01	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	181	GTP	N3-C2-N1	-4.99	120.17	127.46
3	C	181	GTP	C5-C6-N1	-2.82	119.47	123.48
3	C	181	GTP	C4'-O4'-C1'	2.16	112.07	109.77
3	C	181	GTP	C6-N1-C2	2.66	119.88	116.06
3	C	181	GTP	C2-N3-C4	4.48	120.39	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	181	GTP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	173/182 (95%)	-0.21	1 (0%)	89 90	94, 135, 186, 331	2 (1%)
2	A	1026/1073 (95%)	-0.31	5 (0%)	90 92	85, 148, 211, 302	1 (0%)
All	All	1199/1255 (95%)	-0.29	6 (0%)	90 92	85, 146, 210, 331	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	401	ASP	3.5
1	C	180	PRO	3.0
2	A	1028	GLU	2.6
2	A	532	ARG	2.1
2	A	678	ILE	2.0
2	A	276	VAL	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, 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	GTP	C	181	32/32	0.94	0.15	-0.55	69,135,151,154	0
4	MG	C	182	1/1	0.90	0.18	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.