Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:38 PM GMT

PDB ID	:	5DIS
Title	:	Crystal structure of a CRM1-RanGTP-SPN1 export complex bound to a 113 amino acid FG-repeat containing fragment of Nup214
Authors	:	Monecke, T.; Port, S.A.; Dickmanns, A.; Kehlenbach, R.H.; Ficner, R.
Deposited on	:	2015-09-01
Resolution	:	2.85 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:

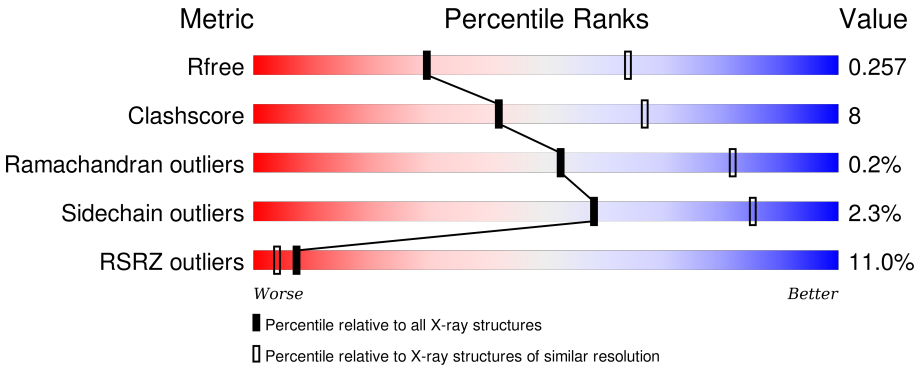
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	1044	% 79% 20% •
2	B	172	% 85% 14% •
3	C	289	3% 67% 23% • 9%
4	D	479	39% 63% 17% • 18%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PRO	A	1101	-	-	-	X
5	PRO	C	301	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14991 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 Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	0	0
			8366	5370	1400	1541	55			

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1398	909	245	239	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	0	0
			2131	1359	365	393	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	linker	UNP O95149
C	0	SER	-	linker	UNP O95149

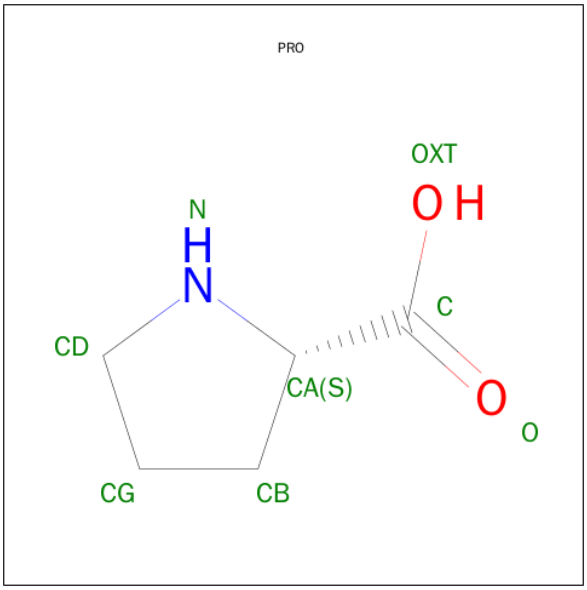
- Molecule 4 is a protein called Maltose-binding periplasmic protein,Nuclear pore complex protein Nup214.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	395	Total	C	N	O	S	0	0	0
			3012	1941	489	579	3			

There are 11 discrepancies between the modelled and reference sequences:

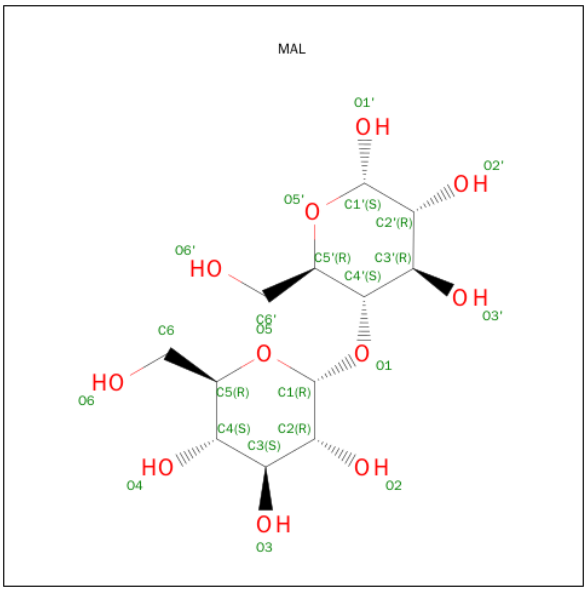
Chain	Residue	Modelled	Actual	Comment	Reference
D	362	ALA	-	linker	UNP P0AEX9
D	363	ALA	-	linker	UNP P0AEX9
D	364	ALA	-	linker	UNP P0AEX9
D	365	GLN	-	linker	UNP P0AEX9
D	366	THR	-	linker	UNP P0AEX9
D	367	ASN	-	linker	UNP P0AEX9
D	368	ALA	-	linker	UNP P0AEX9
D	1912	ALA	-	linker	UNP P0AEX9
D	1913	ALA	-	linker	UNP P0AEX9
D	1914	GLU	-	linker	UNP P0AEX9
D	1915	PHE	-	linker	UNP P0AEX9

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



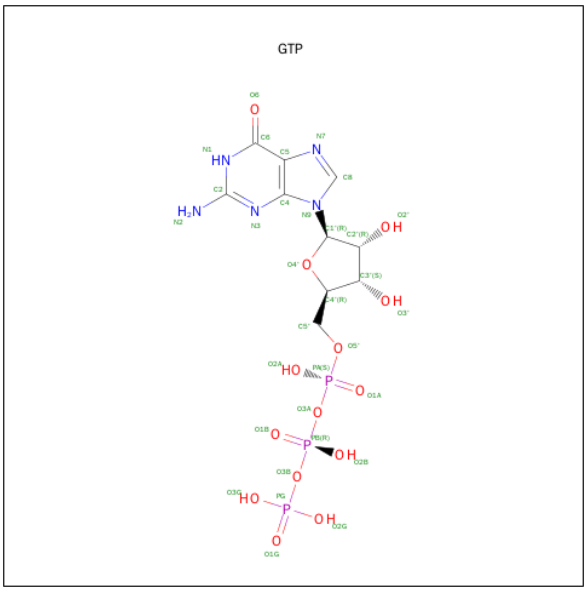
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	5	1	2		
5	C	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 6 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	23	12	11	0	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0

- Molecule 9 is water.

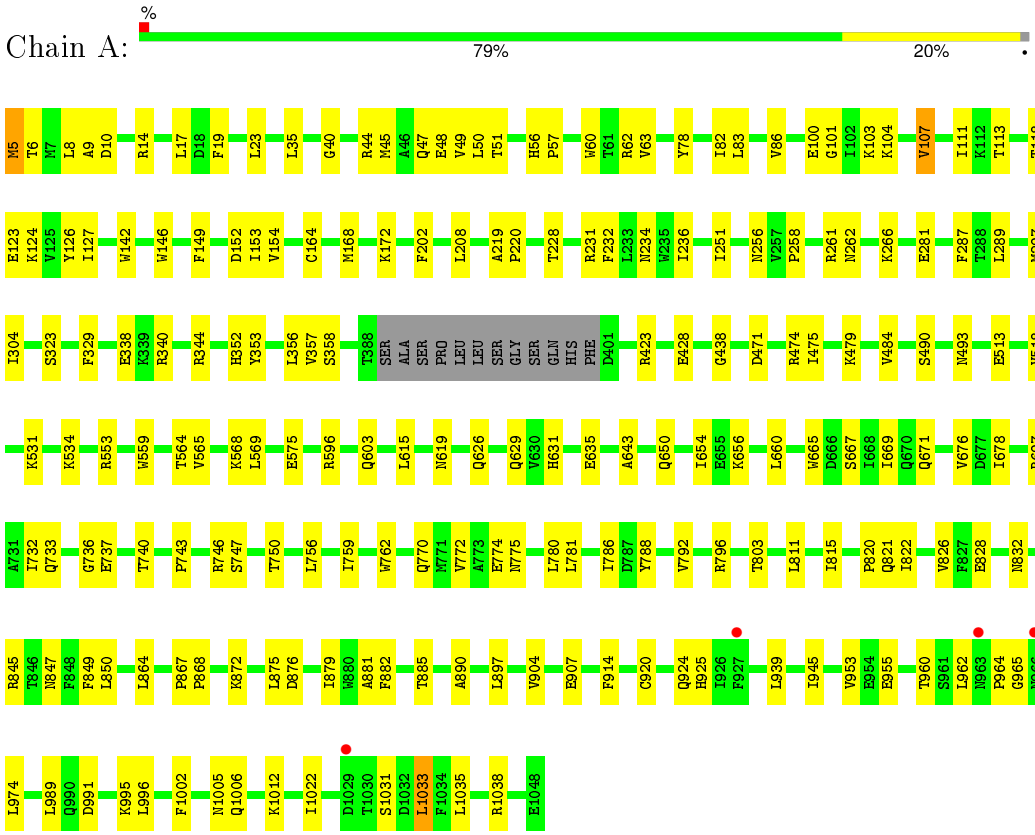
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total O 3 3	0	0
9	B	9	Total O 9 9	0	0

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.

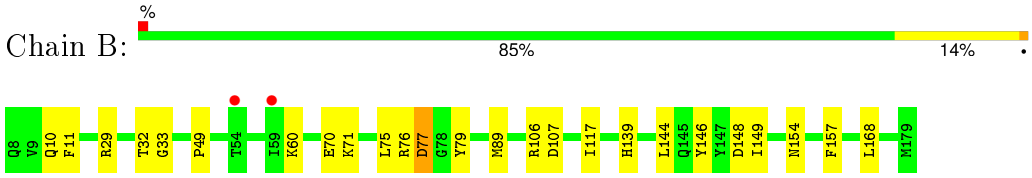
- Molecule 1: Exportin-1

Chain A:



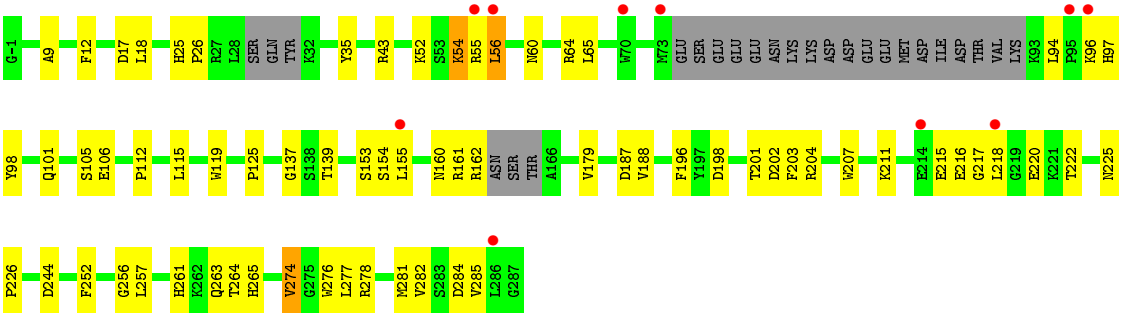
- Molecule 2: GTP-binding nuclear protein Ran

Chain B:



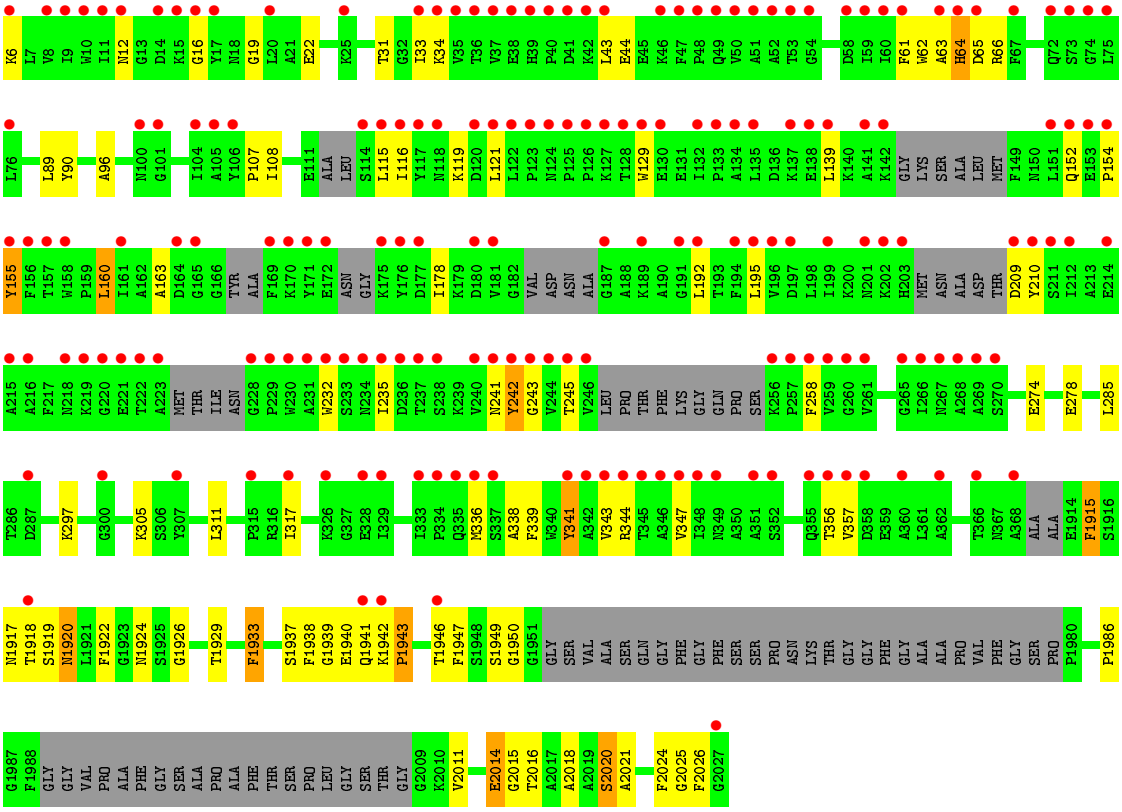
- Molecule 3: Snurportin-1

Chain C:



• Molecule 4: Maltose-binding periplasmic protein,Nuclear pore complex protein Nup214

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	112.33Å 248.97Å 210.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.85 48.49 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.48-2.85) 98.3 (48.49-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.206 , 0.249 0.217 , 0.257	Depositor DCC
R_{free} test set	3396 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 97.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 67922 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14991	wwPDB-VP
Average B, all atoms (Å^2)	125.0	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.*

[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: GTP, MG, MAL

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	0.33	0/8537	0.48	0/11566
2	B	0.35	0/1432	0.48	0/1932
3	C	0.30	0/2186	0.48	0/2957
4	D	0.32	0/3080	0.49	0/4158
All	All	0.32	0/15235	0.48	0/20613

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	8366	0	8417	139	0
2	B	1398	0	1425	15	0
3	C	2131	0	2083	44	0
4	D	3012	0	2923	68	0
5	A	8	0	7	0	0
5	C	8	0	7	1	0
6	A	23	0	22	1	0
7	B	32	0	12	0	0
8	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	3	0	0	1	0
9	B	9	0	0	0	0
All	All	14991	0	14896	251	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 8.

All (251) 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)
4:D:338:ALA:HA	4:D:341:TYR:CE2	2.12	0.84
4:D:2018:ALA:O	4:D:2021:ALA:HB3	1.83	0.78
4:D:155:TYR:HE2	4:D:258:PHE:CE1	2.02	0.77
1:A:251:ILE:HG21	1:A:289:LEU:HB3	1.67	0.77
1:A:471:ASP:OD1	1:A:474:ARG:NH2	2.23	0.72
1:A:19:PHE:HA	1:A:62:ARG:NH2	2.05	0.71
1:A:953:VAL:HG21	1:A:974:LEU:HD11	1.73	0.70
4:D:64:HIS:CE1	4:D:96:ALA:HB1	2.27	0.69
3:C:160:ASN:OD1	3:C:161:ARG:N	2.26	0.69
4:D:2016:THR:O	4:D:2020:SER:OG	2.12	0.68
4:D:339:PHE:O	4:D:343:VAL:HG23	1.94	0.68
1:A:23:LEU:HD22	1:A:62:ARG:HD3	1.76	0.67
4:D:1918:THR:OG1	4:D:1919:SER:N	2.25	0.67
3:C:137:GLY:HA2	3:C:160:ASN:O	1.94	0.67
3:C:65:LEU:HD21	3:C:101:GLN:HE21	1.61	0.66
1:A:358:SER:O	1:A:423:ARG:NH1	2.29	0.65
2:B:70:GLU:O	2:B:76:ARG:NH2	2.30	0.65
1:A:123:GLU:HB2	1:A:126:TYR:HB3	1.79	0.65
4:D:356:THR:HG22	4:D:357:VAL:H	1.61	0.65
1:A:338:GLU:O	1:A:344:ARG:NH2	2.30	0.65
1:A:23:LEU:HB2	1:A:62:ARG:NH1	2.11	0.64
1:A:820:PRO:HB3	4:D:1938:PHE:O	1.97	0.63
4:D:152:GLN:O	4:D:344:ARG:HG3	1.98	0.62
4:D:155:TYR:CE2	4:D:258:PHE:CE1	2.86	0.62
1:A:56:HIS:CD2	1:A:57:PRO:HD2	2.34	0.62
1:A:9:ALA:HA	1:A:49:VAL:HG22	1.80	0.62
4:D:343:VAL:O	4:D:347:VAL:HG23	1.99	0.61
2:B:49:PRO:HB3	2:B:60:LYS:HE2	1.81	0.61
1:A:103:LYS:O	1:A:107:VAL:HG13	2.00	0.61
3:C:54:LYS:HD2	3:C:198:ASP:OD1	2.00	0.61
4:D:258:PHE:O	4:D:258:PHE:CD1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:O	1:A:479:LYS:HG2	1.99	0.61
1:A:840:GLU:O	1:A:845:ARG:NH1	2.33	0.60
4:D:2014:GLU:OE1	4:D:2015:GLY:N	2.35	0.60
1:A:5:MET:SD	1:A:6:THR:N	2.72	0.60
1:A:6:THR:HA	1:A:9:ALA:HB3	1.84	0.60
4:D:61:PHE:HE1	4:D:108:ILE:HG13	1.67	0.59
4:D:31:THR:HG22	4:D:33:ILE:HG13	1.84	0.59
1:A:864:LEU:HD11	1:A:907:GLU:HG3	1.85	0.59
1:A:955:GLU:OE1	1:A:955:GLU:N	2.35	0.59
1:A:100:GLU:O	1:A:104:LYS:HG3	2.03	0.59
1:A:733:GLN:HG3	1:A:792:VAL:HG21	1.84	0.59
2:B:10:GLN:HB3	2:B:60:LYS:HB3	1.84	0.58
4:D:154:PRO:HD3	4:D:344:ARG:HB2	1.85	0.58
1:A:939:LEU:HG	1:A:1012:LYS:HG3	1.86	0.58
3:C:155:LEU:HG	3:C:225:ASN:HB2	1.86	0.57
1:A:756:LEU:HB3	1:A:803:THR:HG21	1.85	0.57
1:A:231:ARG:O	1:A:234:ASN:HB2	2.05	0.57
1:A:828:GLU:O	1:A:832:ASN:ND2	2.38	0.57
1:A:8:LEU:HD22	1:A:45:MET:SD	2.45	0.57
4:D:274:GLU:O	4:D:278:GLU:HG2	2.05	0.57
1:A:231:ARG:NH2	9:A:1202:HOH:O	2.37	0.57
3:C:278:ARG:HB2	3:C:281:MET:HG3	1.87	0.56
3:C:277:LEU:HD21	3:C:285:VAL:HG21	1.88	0.56
1:A:925:HIS:HA	4:D:1986:PRO:HB3	1.86	0.55
4:D:1949:SER:OG	4:D:1950:GLY:N	2.40	0.55
2:B:106:ARG:HG3	2:B:107:ASP:N	2.20	0.55
4:D:116:ILE:HD11	4:D:232:TRP:CD1	2.42	0.55
1:A:298:LEU:O	1:A:353:TYR:OH	2.18	0.55
4:D:16:GLY:HA2	4:D:297:LYS:HD2	1.89	0.55
1:A:60:TRP:CG	1:A:86:VAL:HG21	2.43	0.55
1:A:837:ASP:O	1:A:845:ARG:NH2	2.40	0.54
4:D:64:HIS:ND1	4:D:96:ALA:HB1	2.22	0.54
1:A:153:ILE:HG22	4:D:2024:PHE:CG	2.43	0.54
1:A:484:VAL:HA	1:A:527:LEU:HD13	1.90	0.54
3:C:155:LEU:HG	3:C:225:ASN:CB	2.38	0.53
1:A:615:LEU:HB3	1:A:656:LYS:HD2	1.90	0.53
1:A:113:THR:HG23	1:A:122:LYS:HE3	1.91	0.53
4:D:6:LYS:HD2	4:D:34:LYS:HD2	1.91	0.53
1:A:438:GLY:N	1:A:746:ARG:HD3	2.24	0.53
1:A:619:ASN:HB2	1:A:660:LEU:HD21	1.91	0.52
1:A:281:GLU:OE2	1:A:340:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:HIS:CD2	3:C:263:GLN:H	2.26	0.52
1:A:152:ASP:HB3	4:D:2025:GLY:H	1.75	0.52
1:A:60:TRP:HB3	1:A:86:VAL:HG21	1.92	0.52
2:B:77:ASP:N	2:B:77:ASP:OD1	2.42	0.52
1:A:1033:LEU:HD12	1:A:1033:LEU:H	1.75	0.52
1:A:19:PHE:HA	1:A:62:ARG:HH21	1.71	0.51
4:D:192:LEU:HD23	4:D:357:VAL:HG13	1.91	0.51
4:D:89:LEU:HD13	4:D:107:PRO:HG2	1.91	0.51
4:D:235:ILE:HG22	4:D:235:ILE:O	2.09	0.51
3:C:276:TRP:CE3	5:C:301:PRO:HG3	2.46	0.51
4:D:108:ILE:HD13	4:D:285:LEU:HD21	1.93	0.51
3:C:60:ASN:O	3:C:64:ARG:HG3	2.11	0.50
4:D:336:MET:O	4:D:339:PHE:HB3	2.11	0.50
1:A:40:GLY:O	1:A:44:ARG:HB2	2.11	0.50
1:A:17:LEU:HD13	1:A:56:HIS:ND1	2.27	0.50
2:B:139:HIS:HB2	2:B:144:LEU:HB2	1.92	0.50
1:A:953:VAL:HG11	1:A:974:LEU:HD12	1.93	0.50
1:A:287:PHE:HB2	1:A:329:PHE:CZ	2.46	0.50
1:A:882:PHE:HA	1:A:890:ALA:HA	1.93	0.50
4:D:235:ILE:HG21	4:D:242:TYR:HD2	1.75	0.50
4:D:339:PHE:CE2	4:D:343:VAL:HG21	2.47	0.50
4:D:119:LYS:HE3	4:D:243:GLY:HA3	1.93	0.49
4:D:119:LYS:HB2	4:D:241:ASN:HB3	1.94	0.49
1:A:732:ILE:O	1:A:736:GLY:N	2.45	0.49
3:C:257:LEU:HD12	3:C:282:VAL:HG21	1.94	0.49
1:A:811:LEU:HD12	1:A:815:ILE:HD12	1.93	0.49
1:A:879:ILE:HA	1:A:882:PHE:CE2	2.47	0.49
3:C:202:ASP:OD1	3:C:203:PHE:N	2.46	0.49
1:A:991:ASP:O	1:A:995:LYS:HG2	2.12	0.49
1:A:568:LYS:HE2	3:C:12:PHE:HB3	1.95	0.49
4:D:338:ALA:HA	4:D:341:TYR:CD2	2.47	0.48
1:A:60:TRP:HA	1:A:63:VAL:HG23	1.95	0.48
1:A:78:TYR:CE2	1:A:82:ILE:HD11	2.48	0.48
1:A:438:GLY:H	1:A:746:ARG:HD3	1.78	0.48
1:A:676:VAL:HG12	4:D:1922:PHE:HB2	1.95	0.48
1:A:202:PHE:CZ	1:A:236:ILE:HG21	2.49	0.48
1:A:490:SER:HB3	1:A:493:ASN:OD1	2.14	0.48
1:A:172:LYS:HB2	1:A:228:THR:HG23	1.95	0.48
4:D:160:LEU:HD23	4:D:163:ALA:HB3	1.96	0.48
3:C:264:THR:HG22	3:C:265:HIS:O	2.14	0.48
2:B:89:MET:CE	2:B:149:ILE:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1915:PHE:N	4:D:1915:PHE:CD1	2.76	0.48
3:C:115:LEU:HD12	3:C:119:TRP:HB2	1.95	0.47
1:A:1002:PHE:O	1:A:1005:ASN:ND2	2.47	0.47
4:D:1920:ASN:OD1	4:D:1920:ASN:N	2.46	0.47
1:A:119:CYS:HA	1:A:122:LYS:HB3	1.95	0.47
1:A:1005:ASN:OD1	1:A:1006:GLN:HG3	2.14	0.47
2:B:32:THR:OG1	2:B:33:GLY:N	2.48	0.47
3:C:201:THR:HG23	3:C:264:THR:O	2.14	0.47
1:A:847:ASN:HA	1:A:850:LEU:HD12	1.95	0.47
3:C:56:LEU:HD12	3:C:56:LEU:N	2.30	0.47
3:C:160:ASN:CG	3:C:162:ARG:HG2	2.35	0.47
3:C:96:LYS:O	3:C:97:HIS:HB2	2.14	0.47
4:D:311:LEU:HB3	4:D:317:ILE:HD12	1.96	0.47
4:D:116:ILE:HD11	4:D:232:TRP:HD1	1.80	0.47
3:C:153:SER:O	3:C:226:PRO:HD2	2.15	0.47
1:A:631:HIS:HB3	1:A:697:ARG:HG3	1.97	0.46
4:D:1939:GLY:C	4:D:1940:GLU:HG3	2.36	0.46
2:B:75:LEU:HD12	2:B:79:TYR:CE1	2.51	0.46
1:A:849:PHE:CE1	1:A:881:ALA:HB2	2.50	0.46
4:D:155:TYR:HE2	4:D:258:PHE:CD1	2.34	0.46
1:A:770:GLN:O	1:A:774:GLU:HG2	2.15	0.46
3:C:105:SER:HB3	3:C:274:VAL:HG22	1.98	0.46
1:A:56:HIS:HD2	1:A:57:PRO:HD2	1.80	0.46
1:A:996:LEU:HD21	1:A:1038:ARG:HG2	1.98	0.46
3:C:207:TRP:CH2	3:C:211:LYS:HD3	2.51	0.46
1:A:8:LEU:HD12	1:A:8:LEU:H	1.81	0.46
1:A:104:LYS:HB3	4:D:2021:ALA:CB	2.46	0.46
1:A:743:PRO:O	1:A:746:ARG:HB3	2.16	0.45
1:A:868:PRO:HG2	4:D:1946:THR:OG1	2.17	0.45
4:D:129:TRP:CZ3	4:D:195:LEU:HD11	2.52	0.45
3:C:215:GLU:C	3:C:216:GLU:HG2	2.36	0.45
1:A:60:TRP:CB	1:A:86:VAL:HG21	2.47	0.45
3:C:55:ARG:N	3:C:56:LEU:HD12	2.31	0.45
3:C:125:PRO:HB3	3:C:252:PHE:CG	2.51	0.45
3:C:217:GLY:HA2	3:C:220:GLU:OE1	2.16	0.45
2:B:117:ILE:HB	2:B:144:LEU:HD22	1.99	0.45
1:A:228:THR:HG22	1:A:232:PHE:CE2	2.51	0.45
2:B:146:TYR:OH	2:B:148:ASP:OD1	2.24	0.45
2:B:11:PHE:CG	2:B:168:LEU:HD13	2.52	0.45
1:A:104:LYS:O	4:D:2021:ALA:HB2	2.16	0.45
1:A:6:THR:O	1:A:10:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:H	1:A:1035:LEU:HD12	1.81	0.45
1:A:596:ARG:HB2	1:A:643:ALA:HB2	1.99	0.45
1:A:759:ILE:HD13	1:A:780:LEU:HD21	1.99	0.45
1:A:872:LYS:NZ	1:A:876:ASP:OD2	2.38	0.45
1:A:727:ASN:HA	4:D:1918:THR:HB	1.99	0.45
4:D:235:ILE:CG2	4:D:242:TYR:HD2	2.30	0.45
3:C:125:PRO:HB3	3:C:252:PHE:CD1	2.52	0.45
3:C:139:THR:OG1	3:C:154:SER:HB3	2.17	0.45
3:C:18:LEU:HD23	3:C:35:TYR:HA	1.99	0.45
4:D:1942:LYS:HA	4:D:1943:PRO:HD3	1.85	0.45
1:A:107:VAL:O	1:A:111:ILE:HG12	2.17	0.44
3:C:198:ASP:O	3:C:265:HIS:NE2	2.49	0.44
1:A:960:THR:HG21	1:A:965:GLY:HA2	1.99	0.44
3:C:196:PHE:O	3:C:204:ARG:HD3	2.17	0.44
1:A:1031:SER:HA	1:A:1033:LEU:CD1	2.47	0.44
1:A:788:TYR:CZ	1:A:796:ARG:HD3	2.52	0.44
1:A:258:PRO:O	1:A:261:ARG:HG2	2.17	0.44
3:C:216:GLU:O	3:C:218:LEU:N	2.49	0.44
1:A:564:THR:HG23	3:C:9:ALA:HB2	1.99	0.44
1:A:490:SER:OG	6:A:1102:MAL:H6'1	2.18	0.44
2:B:89:MET:HE2	2:B:149:ILE:HD11	1.98	0.44
3:C:112:PRO:HG3	3:C:119:TRP:CE2	2.52	0.44
3:C:97:HIS:O	3:C:98:TYR:HB2	2.16	0.44
1:A:304:ILE:HG13	1:A:356:LEU:HB3	2.00	0.44
1:A:35:LEU:HD22	1:A:50:LEU:HD12	1.98	0.44
1:A:63:VAL:HG11	1:A:83:LEU:HD22	2.00	0.44
1:A:897:LEU:HD23	1:A:945:ILE:HD13	1.99	0.44
4:D:62:TRP:CG	4:D:63:ALA:N	2.85	0.44
1:A:635:GLU:OE1	1:A:697:ARG:HD2	2.17	0.44
4:D:65:ASP:OD2	4:D:66:ARG:HG2	2.18	0.44
1:A:534:LYS:NZ	1:A:575:GLU:OE2	2.50	0.44
1:A:730:ALA:HB3	4:D:1918:THR:HG22	1.99	0.43
1:A:146:TRP:CD1	1:A:149:PHE:HB2	2.53	0.43
1:A:565:VAL:O	1:A:569:LEU:HD13	2.18	0.43
3:C:54:LYS:H	3:C:54:LYS:HG2	1.57	0.43
1:A:120:VAL:HG13	1:A:124:LYS:HE3	1.98	0.43
4:D:90:TYR:CE1	4:D:305:LYS:HG2	2.53	0.43
1:A:747:SER:O	1:A:750:THR:HB	2.19	0.43
1:A:667:SER:O	1:A:671:GLN:HG3	2.18	0.43
1:A:172:LYS:HB3	1:A:172:LYS:HE2	1.88	0.43
1:A:518:VAL:O	1:A:522:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:CYS:O	1:A:924:GLN:HG2	2.19	0.43
1:A:123:GLU:O	1:A:127:ILE:HG13	2.19	0.43
3:C:256:GLY:O	3:C:257:LEU:HD23	2.19	0.43
4:D:43:LEU:HD12	4:D:44:GLU:N	2.32	0.43
1:A:154:VAL:HG22	1:A:208:LEU:HD12	2.01	0.43
4:D:115:LEU:HD13	4:D:245:THR:HG23	2.00	0.43
2:B:71:LYS:HE3	2:B:71:LYS:HB2	1.84	0.43
1:A:968:VAL:CG1	1:A:973:PHE:HB2	2.49	0.43
1:A:774:GLU:HG3	1:A:775:ASN:OD1	2.19	0.42
1:A:781:LEU:O	1:A:786:ILE:HG13	2.19	0.42
3:C:43:ARG:NH2	3:C:106:GLU:OE2	2.51	0.42
4:D:1917:ASN:OD1	4:D:1918:THR:N	2.52	0.42
1:A:300:LEU:HB3	1:A:352:HIS:CE1	2.55	0.42
1:A:559:TRP:CD2	1:A:603:GLN:HG3	2.55	0.42
1:A:19:PHE:CA	1:A:62:ARG:HH21	2.32	0.42
4:D:1933:PHE:C	4:D:1933:PHE:CD1	2.92	0.42
1:A:904:VAL:HG11	1:A:914:PHE:CD2	2.53	0.42
4:D:19:GLY:HA2	4:D:22:GLU:CD	2.40	0.42
3:C:55:ARG:H	3:C:56:LEU:HD12	1.85	0.42
4:D:1926:GLY:HA2	4:D:1929:THR:HG22	2.00	0.42
1:A:168:MET:HB3	1:A:168:MET:HE3	1.86	0.42
1:A:626:GLN:HG2	1:A:629:GLN:HG3	2.02	0.42
4:D:155:TYR:CE2	4:D:258:PHE:CD1	3.08	0.42
1:A:118:THR:O	1:A:122:LYS:HB2	2.20	0.42
1:A:256:ASN:HA	1:A:297:MET:SD	2.60	0.42
3:C:25:HIS:HA	3:C:26:PRO:HD3	1.87	0.42
1:A:344:ARG:HA	1:A:344:ARG:HD3	1.75	0.42
1:A:1033:LEU:N	1:A:1033:LEU:HD12	2.33	0.42
3:C:215:GLU:HG3	3:C:215:GLU:O	2.20	0.42
1:A:737:GLU:O	1:A:740:THR:HG22	2.20	0.41
1:A:821:GLN:HG2	1:A:821:GLN:H	1.68	0.41
1:A:104:LYS:HA	4:D:2021:ALA:HB1	2.02	0.41
4:D:1937:SER:O	4:D:1938:PHE:HB2	2.20	0.41
3:C:187:ASP:OD1	3:C:188:VAL:N	2.53	0.41
1:A:531:LYS:HA	1:A:531:LYS:HD3	1.89	0.41
1:A:513:GLU:CD	1:A:553:ARG:HH21	2.23	0.41
1:A:164:CYS:O	1:A:168:MET:HG2	2.20	0.41
3:C:277:LEU:HG	3:C:281:MET:HB2	2.01	0.41
1:A:650:GLN:O	1:A:654:ILE:HG13	2.20	0.41
1:A:262:ASN:O	1:A:266:LYS:HG3	2.20	0.41
1:A:219:ALA:HB3	1:A:220:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HG11	1:A:146:TRP:HH2	1.86	0.41
1:A:142:TRP:HD1	1:A:146:TRP:O	2.04	0.41
1:A:867:PRO:HA	1:A:868:PRO:HD3	1.84	0.41
1:A:665:TRP:O	1:A:669:ILE:HG12	2.21	0.41
1:A:822:ILE:O	1:A:826:VAL:HG22	2.21	0.41
1:A:101:GLY:HA3	4:D:2011:VAL:HG13	2.03	0.41
1:A:762:TRP:CH2	1:A:772:VAL:HG22	2.55	0.41
1:A:962:LEU:HB3	1:A:964:PRO:HD2	2.02	0.41
4:D:209:ASP:OD1	4:D:210:TYR:N	2.50	0.41
1:A:323:SER:HB3	1:A:357:VAL:HG11	2.03	0.41
1:A:104:LYS:CA	4:D:2021:ALA:HB1	2.51	0.41
1:A:953:VAL:HG21	1:A:974:LEU:CD1	2.48	0.41
4:D:121:LEU:HB3	4:D:139:LEU:HD11	2.02	0.41
1:A:44:ARG:O	1:A:48:GLU:HG3	2.21	0.40
2:B:29:ARG:HG2	2:B:157:PHE:CZ	2.57	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	1028/1044 (98%)	983 (96%)	45 (4%)	0	100	100
2	B	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
3	C	256/289 (89%)	241 (94%)	15 (6%)	0	100	100
4	D	371/479 (78%)	334 (90%)	34 (9%)	3 (1%)	24	56
All	All	1825/1984 (92%)	1720 (94%)	102 (6%)	3 (0%)	52	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1941	GLN
4	D	1933	PHE
4	D	1943	PRO

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	941/951 (99%)	929 (99%)	12 (1%)	76 92
2	B	151/151 (100%)	149 (99%)	2 (1%)	76 92
3	C	237/262 (90%)	227 (96%)	10 (4%)	36 70
4	D	304/360 (84%)	290 (95%)	14 (5%)	33 66
All	All	1633/1724 (95%)	1595 (98%)	38 (2%)	58 85

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	14	ARG
1	A	47	GLN
1	A	51	THR
1	A	107	VAL
1	A	428	GLU
1	A	678	ILE
1	A	875	LEU
1	A	885	THR
1	A	989	LEU
1	A	1022	ILE
1	A	1033	LEU
2	B	77	ASP
2	B	154	ASN
3	C	17	ASP
3	C	52	LYS
3	C	54	LYS
3	C	56	LEU
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	179	VAL
3	C	222	THR
3	C	244	ASP
3	C	274	VAL
3	C	284	ASP
4	D	12	ASN
4	D	64	HIS
4	D	155	TYR
4	D	160	LEU
4	D	178	ILE
4	D	242	TYR
4	D	341	TYR
4	D	1915	PHE
4	D	1920	ASN
4	D	1924	ASN
4	D	1947	PHE
4	D	2014	GLU
4	D	2020	SER
4	D	2026	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	101	GLN
3	C	261	HIS

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	PRO	A	1101	-	4,8,8	0.48	0	5,10,10	1.08	0
6	MAL	A	1102	-	24,24,24	0.43	0	35,35,35	1.63	4 (11%)
7	GTP	B	201	8	26,34,34	1.13	2 (7%)	29,54,54	1.85	4 (13%)
5	PRO	C	301	-	4,8,8	0.47	0	5,10,10	1.08	1 (20%)

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
5	PRO	A	1101	-	-	0/0/11/11	0/1/1/1
6	MAL	A	1102	-	-	0/8/48/48	0/2/2/2
7	GTP	B	201	8	-	0/18/38/38	0/3/3/3
5	PRO	C	301	-	-	0/0/11/11	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	201	GTP	C5-C4	2.48	1.46	1.40
7	B	201	GTP	C6-C5	3.32	1.48	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	201	GTP	C5-C6-N1	-4.50	117.64	123.52
7	B	201	GTP	N3-C2-N1	-3.74	122.47	127.56
7	B	201	GTP	C6-C5-C4	-3.19	117.21	120.86
5	C	301	PRO	CD-N-CA	2.05	112.15	107.07
6	A	1102	MAL	C3-C4-C5	3.16	115.86	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1102	MAL	C1-O5-C5	4.39	122.35	113.74
6	A	1102	MAL	O5-C5-C4	4.47	118.20	109.67
6	A	1102	MAL	O1-C4'-C3'	4.74	119.54	107.18
7	B	201	GTP	C6-N1-C2	5.64	122.49	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1102	MAL	1	0
5	C	301	PRO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1032/1044 (98%)	0.00	6 (0%) 90 89	59, 92, 145, 259	0
2	B	172/172 (100%)	0.06	2 (1%) 81 78	57, 83, 128, 204	0
3	C	264/289 (91%)	0.08	10 (3%) 44 37	72, 125, 190, 230	0
4	D	395/479 (82%)	2.36	187 (47%) 0 0	109, 213, 281, 329	0
All	All	1863/1984 (93%)	0.52	205 (11%) 7 4	57, 105, 246, 329	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	346	ALA	19.6
4	D	348	ILE	11.2
4	D	234	ASN	11.1
4	D	201	ASN	10.6
4	D	115	LEU	10.4
4	D	345	THR	10.0
4	D	116	ILE	9.6
4	D	176	TYR	9.2
4	D	152	GLN	8.4
4	D	74	GLY	8.4
4	D	43	LEU	8.3
4	D	221	GLU	8.1
4	D	121	LEU	8.0
4	D	210	TYR	8.0
4	D	151	LEU	7.9
4	D	220	GLY	7.5
4	D	134	ALA	7.1
4	D	40	PRO	7.1
4	D	237	THR	7.0
4	D	9	ILE	7.0
4	D	211	SER	6.9

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Mol	Chain	Res	Type	RSRZ
4	D	16	GLY	6.9
4	D	334	PRO	6.8
4	D	135	LEU	6.5
4	D	35	VAL	6.4
4	D	15	LYS	6.4
4	D	114	SER	6.3
4	D	222	THR	6.3
4	D	260	GLY	6.2
4	D	266	ILE	6.2
4	D	124	ASN	6.2
4	D	47	PHE	6.1
1	A	967	PRO	6.1
4	D	141	ALA	6.1
4	D	333	ILE	6.0
4	D	244	VAL	6.0
4	D	233	SER	5.9
4	D	11	ILE	5.8
4	D	259	VAL	5.4
4	D	153	GLU	5.3
4	D	242	TYR	5.3
4	D	122	LEU	5.3
4	D	238	SER	5.3
4	D	72	GLN	5.3
4	D	357	VAL	5.3
4	D	337	SER	5.2
4	D	356	THR	5.2
3	C	55	ARG	5.1
4	D	123	PRO	5.0
4	D	197	ASP	5.0
4	D	362	ALA	5.0
4	D	241	ASN	5.0
4	D	214	GLU	4.9
4	D	17	TYR	4.9
3	C	96	LYS	4.8
4	D	368	ALA	4.8
4	D	328	GLU	4.7
4	D	209	ASP	4.7
3	C	73	MET	4.7
4	D	229	PRO	4.7
4	D	347	VAL	4.7
4	D	181	VAL	4.7
4	D	61	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
4	D	53	THR	4.6
4	D	41	ASP	4.6
4	D	2027	GLY	4.5
4	D	358	ASP	4.5
4	D	261	VAL	4.5
4	D	158	TRP	4.5
4	D	8	VAL	4.4
3	C	286	LEU	4.4
4	D	12	ASN	4.4
4	D	75	LEU	4.3
4	D	228	GLY	4.3
4	D	120	ASP	4.3
4	D	170	LYS	4.3
4	D	1918	THR	4.3
4	D	349	ASN	4.2
4	D	73	SER	4.2
4	D	132	ILE	4.2
4	D	54	GLY	4.2
4	D	125	PRO	4.1
4	D	64	HIS	4.1
4	D	101	GLY	4.1
4	D	317	ILE	4.1
4	D	117	TYR	4.1
4	D	10	TRP	4.1
4	D	39	HIS	4.0
4	D	246	VAL	4.0
4	D	118	ASN	4.0
4	D	137	LYS	4.0
4	D	129	TRP	3.9
4	D	133	PRO	3.9
3	C	56	LEU	3.8
4	D	127	LYS	3.8
4	D	223	ALA	3.8
4	D	165	GLY	3.8
4	D	59	ILE	3.8
4	D	216	ALA	3.7
4	D	355	GLN	3.7
4	D	218	ASN	3.7
4	D	267	ASN	3.7
4	D	195	LEU	3.7
4	D	67	PHE	3.6
4	D	352	SER	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	130	GLU	3.6
1	A	1029	ASP	3.5
2	B	59	ILE	3.4
4	D	157	THR	3.4
4	D	231	ALA	3.4
4	D	139	LEU	3.4
4	D	187	GLY	3.4
4	D	50	VAL	3.4
4	D	245	THR	3.4
4	D	138	GLU	3.3
4	D	154	PRO	3.3
1	A	121	GLU	3.3
4	D	36	THR	3.3
4	D	42	LYS	3.3
4	D	52	ALA	3.2
4	D	104	ILE	3.2
4	D	172	GLU	3.2
4	D	58	ASP	3.2
4	D	38	GLU	3.2
1	A	966	ASN	3.1
4	D	100	ASN	3.1
4	D	194	PHE	3.1
1	A	963	ASN	3.1
4	D	236	ASP	3.1
4	D	342	ALA	3.1
4	D	235	ILE	3.1
4	D	1946	THR	3.1
4	D	315	PRO	3.0
4	D	142	LYS	3.0
4	D	155	TYR	3.0
3	C	95	PRO	3.0
4	D	63	ALA	3.0
4	D	202	LYS	3.0
4	D	1942	LYS	3.0
4	D	344	ARG	2.9
4	D	269	ALA	2.9
4	D	164	ASP	2.9
4	D	300	GLY	2.9
4	D	243	GLY	2.9
4	D	329	ILE	2.9
4	D	258	PHE	2.9
4	D	20	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	105	ALA	2.8
4	D	287	ASP	2.8
4	D	48	PRO	2.8
4	D	34	LYS	2.8
4	D	76	LEU	2.7
4	D	351	ALA	2.7
4	D	65	ASP	2.7
4	D	51	ALA	2.7
4	D	199	ILE	2.7
4	D	175	LYS	2.7
4	D	33	ILE	2.6
4	D	60	ILE	2.6
4	D	192	LEU	2.5
4	D	1941	GLN	2.5
4	D	191	GLY	2.5
4	D	37	VAL	2.5
4	D	25	LYS	2.5
4	D	265	GLY	2.5
3	C	70	TRP	2.5
4	D	366	THR	2.5
4	D	171	TYR	2.5
4	D	268	ALA	2.4
4	D	335	GLN	2.4
4	D	161	ILE	2.4
4	D	203	HIS	2.4
1	A	927	PHE	2.4
4	D	106	TYR	2.4
4	D	156	PHE	2.4
4	D	240	VAL	2.4
4	D	343	VAL	2.4
4	D	232	TRP	2.4
4	D	212	ILE	2.4
4	D	126	PRO	2.3
3	C	155	LEU	2.3
2	B	54	THR	2.3
4	D	219	LYS	2.3
4	D	256	LYS	2.3
4	D	46	LYS	2.3
4	D	307	TYR	2.3
4	D	230	TRP	2.2
4	D	14	ASP	2.2
4	D	270	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	214	GLU	2.2
4	D	189	LYS	2.2
4	D	177	ASP	2.2
4	D	215	ALA	2.2
4	D	128	THR	2.2
4	D	196	VAL	2.2
4	D	341	TYR	2.2
4	D	336	MET	2.1
4	D	180	ASP	2.1
4	D	169	PHE	2.1
4	D	257	PRO	2.1
4	D	49	GLN	2.1
4	D	326	LYS	2.1
3	C	218	LEU	2.1
4	D	6	LYS	2.1
4	D	360	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
5	PRO	C	301	8/8	0.76	0.72	15.45	166,188,275,329	0
5	PRO	A	1101	8/8	0.80	0.30	4.52	122,126,137,140	0
7	GTP	B	201	32/32	0.95	0.16	-0.51	56,75,106,135	0
8	MG	B	202	1/1	0.86	0.14	-0.52	94,94,94,94	0
6	MAL	A	1102	23/23	0.73	0.32	-	153,193,235,236	0

6.5 Other polymers (i)

There are no such residues in this entry.