Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:38 am GMT

PDB ID	:	2XO5
Title	:	RIBONUCLEOTIDE REDUCTASE Y731NH2Y MODIFIED R1 SUBUNIT OF E. COLI
Authors	:	Minnihan, E.C.; Seyedsayamdost, M.R.; Uhlin, U.; Stubbe, J.
Deposited on	:	2010-08-09
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

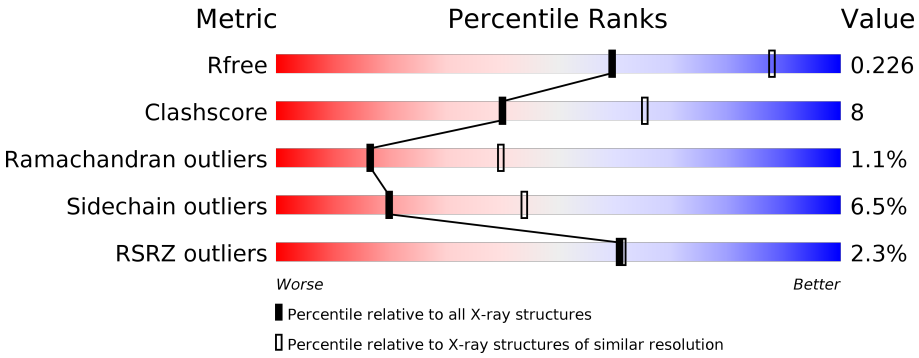
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	761	3% 78% 17%
1	B	761	2% 76% 19%
1	C	761	% 78% 16%
2	D	20	15% 65% 10% 5% 20%
2	E	20	10% 65% 15% 20%
2	F	20	10% 60% 15% 5% 20%

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Mol	Chain	Length	Quality of chain
2	P	20	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18854 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 RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			
1	B	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			
1	C	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	E	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	F	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	274	Total	O	0	0
			274	274		
3	B	256	Total	O	0	0
			256	256		
3	C	354	Total	O	0	0
			354	354		
3	D	5	Total	O	0	0
			5	5		

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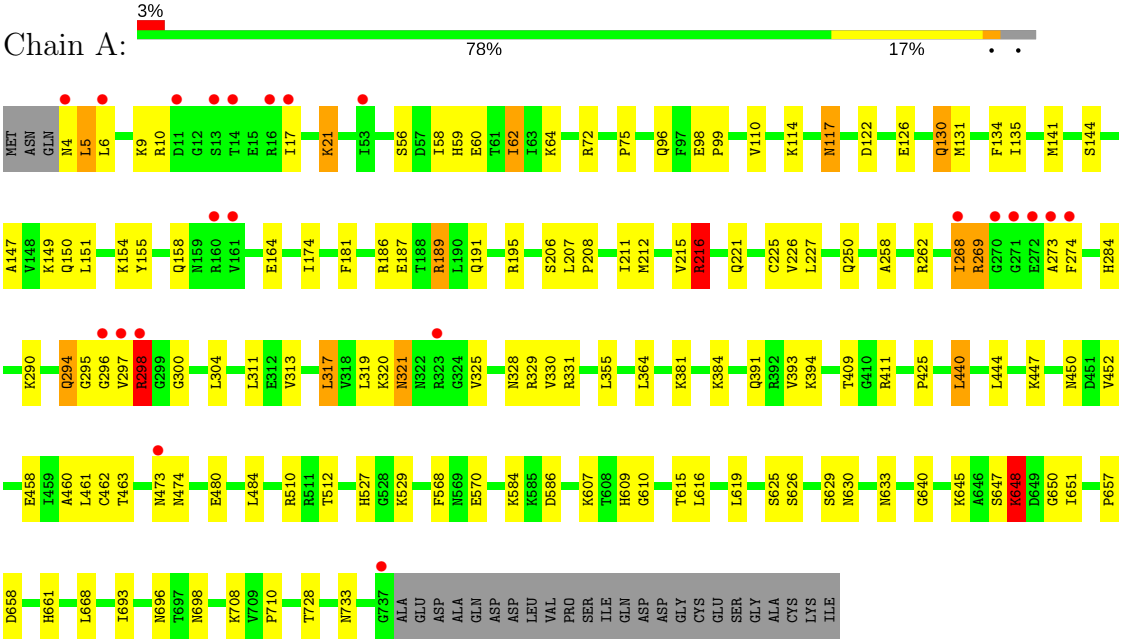
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	4	Total O 4 4	0	0
3	F	4	Total O 4 4	0	0
3	P	5	Total O 5 5	0	0

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 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.

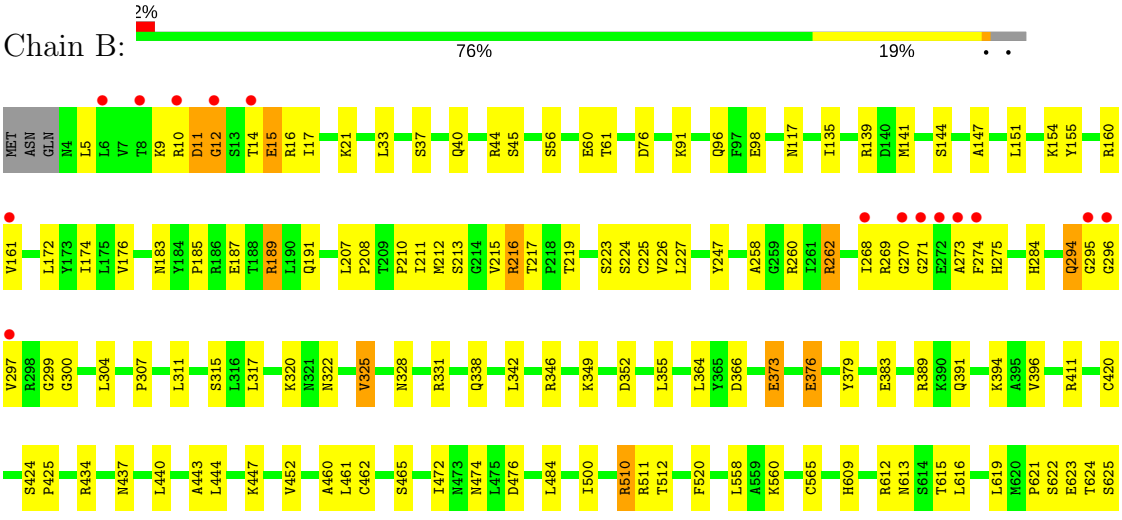
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

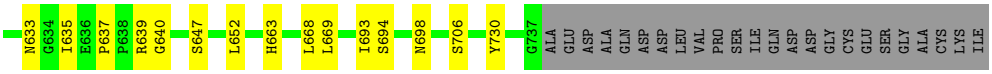
Chain A:



• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

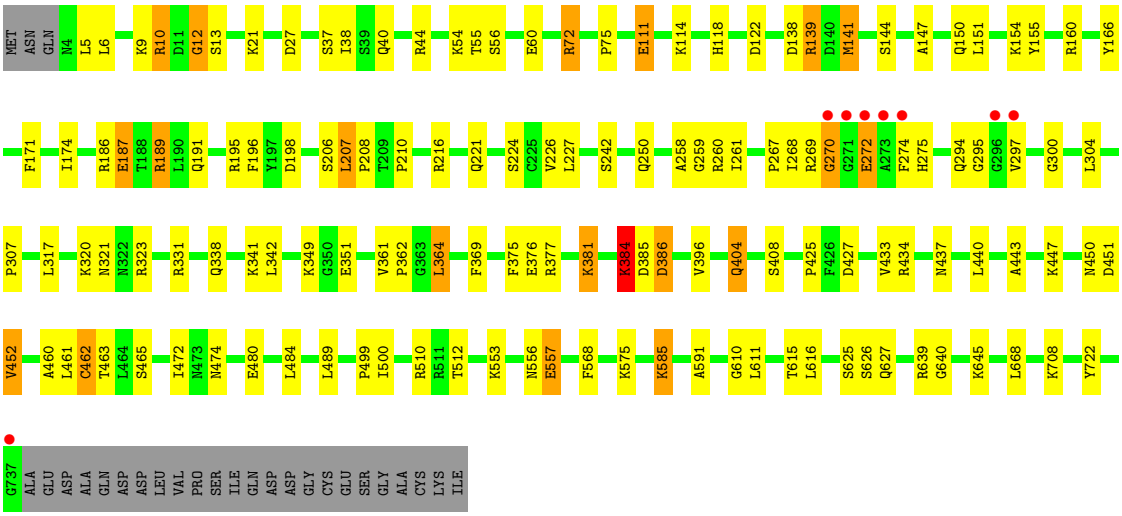
Chain B:





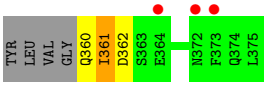
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C:



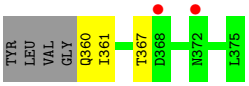
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain D:



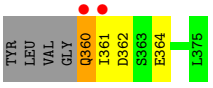
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain E:



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain F:



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	223.24Å 223.24Å 335.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	166.67 – 2.70 79.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (166.67-2.70) 99.9 (79.02-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.228 0.176 , 0.226	Depositor DCC
R_{free} test set	4408 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18854	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.333 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: TY2

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	0.47	0/5959	0.59	0/8069
1	B	0.46	0/5959	0.59	0/8069
1	C	0.51	1/5959 (0.0%)	0.62	0/8069
2	D	0.50	0/129	0.61	0/173
2	E	0.43	0/129	0.61	0/173
2	F	0.44	0/129	0.69	0/173
2	P	0.63	0/27	0.63	0/36
All	All	0.48	1/18291 (0.0%)	0.60	0/24762

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	462	CYS	CB-SG	5.09	1.91	1.82

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	5846	0	5770	96	0
1	B	5846	0	5770	97	0
1	C	5846	0	5769	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	129	0	111	3	0
2	E	129	0	111	0	0
2	F	129	0	111	2	0
2	P	27	0	31	3	0
3	A	274	0	0	34	0
3	B	256	0	0	31	2
3	C	354	0	0	45	1
3	D	5	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	P	5	0	0	3	0
All	All	18854	0	17673	295	2

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 (295) 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:C:450:ASN:HB2	3:C:2230:HOH:O	1.37	1.22
1:C:191:GLN:HB2	3:C:2099:HOH:O	1.50	1.12
1:C:331:ARG:HD2	3:C:2169:HOH:O	1.51	1.10
1:B:117:ASN:HB2	3:B:2049:HOH:O	1.59	1.02
1:B:225:CYS:HB3	3:B:2151:HOH:O	1.60	1.01
1:C:111:GLU:HG2	3:C:2060:HOH:O	1.59	1.01
1:A:221:GLN:HE22	1:B:271:GLY:HA3	1.32	0.93
1:B:225:CYS:CB	3:B:2151:HOH:O	2.15	0.92
1:C:480:GLU:HB3	3:C:2105:HOH:O	1.70	0.90
1:C:272:GLU:HG2	3:C:2145:HOH:O	1.70	0.90
1:C:611:LEU:HD23	3:C:2291:HOH:O	1.72	0.88
1:C:195:ARG:HD3	3:C:2104:HOH:O	1.75	0.85
1:A:215:VAL:O	1:A:216:ARG:HB3	1.78	0.82
1:C:556:ASN:HA	3:C:2291:HOH:O	1.82	0.79
1:B:208:PRO:HG2	1:B:211:ILE:HD12	1.66	0.78
1:B:262:ARG:HD3	1:B:274:PHE:HB3	1.63	0.78
1:C:27:ASP:HA	1:C:38:ILE:HD11	1.66	0.78
1:C:122:ASP:O	1:C:189:ARG:NH2	2.19	0.76
1:A:187:GLU:OE1	1:C:186:ARG:HG3	1.84	0.76
1:B:268:ILE:HA	3:B:2098:HOH:O	1.84	0.75
1:C:191:GLN:HG3	3:C:2100:HOH:O	1.85	0.74
1:C:12:GLY:HA2	3:C:2011:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ARG:HA	3:C:2083:HOH:O	1.89	0.72
1:B:215:VAL:O	1:B:216:ARG:HB3	1.88	0.72
1:B:262:ARG:HD3	1:B:274:PHE:CB	2.19	0.72
1:B:91:LYS:HE3	3:B:2040:HOH:O	1.88	0.72
1:C:450:ASN:CB	3:C:2230:HOH:O	2.10	0.71
1:A:212:MET:O	1:A:216:ARG:NH2	2.24	0.70
1:A:207:LEU:HD13	1:A:212:MET:CE	2.22	0.70
1:B:155:TYR:HE1	3:B:2075:HOH:O	1.74	0.70
1:A:268:ILE:HD11	1:A:273:ALA:HA	1.74	0.69
1:B:268:ILE:HB	1:B:275:HIS:NE2	2.08	0.68
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.25	0.68
1:B:212:MET:O	1:B:216:ARG:NH2	2.26	0.68
1:B:268:ILE:HB	1:B:275:HIS:CE1	2.29	0.68
1:C:155:TYR:HD1	3:C:2110:HOH:O	1.77	0.67
1:B:663:HIS:HD2	3:B:2232:HOH:O	1.77	0.67
1:C:155:TYR:CD1	3:C:2110:HOH:O	2.47	0.67
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.77	0.66
1:B:269:ARG:HA	3:B:2092:HOH:O	1.96	0.66
1:C:274:PHE:CD2	3:C:2139:HOH:O	2.49	0.65
1:A:226:VAL:HG12	1:A:461:LEU:HD23	1.77	0.65
1:A:207:LEU:HD13	1:A:212:MET:HE1	1.78	0.65
1:C:44:ARG:HD3	3:C:2026:HOH:O	1.97	0.65
1:B:154:LYS:HD2	1:B:624:THR:HG21	1.78	0.64
1:C:404:GLN:HB2	2:F:361:ILE:HD13	1.80	0.64
1:A:480:GLU:HB3	3:A:2086:HOH:O	1.97	0.64
1:B:14:THR:O	1:B:15:GLU:HB2	1.97	0.64
1:B:294:GLN:HG2	3:B:2104:HOH:O	1.98	0.63
1:A:191:GLN:HB2	3:A:2084:HOH:O	1.98	0.62
1:C:226:VAL:HG12	1:C:461:LEU:HD23	1.80	0.62
1:B:639:ARG:HD2	3:B:2216:HOH:O	2.00	0.62
1:C:154:LYS:HG3	3:C:2110:HOH:O	1.99	0.62
1:C:639:ARG:HD2	3:C:2310:HOH:O	1.97	0.62
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.81	0.62
1:B:260:ARG:HH21	1:B:434:ARG:HH22	1.48	0.62
1:A:225:CYS:HB3	3:A:2173:HOH:O	1.98	0.62
1:B:191:GLN:HB2	3:B:2069:HOH:O	2.00	0.61
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.82	0.61
1:B:268:ILE:HG21	3:B:2045:HOH:O	1.99	0.61
1:A:268:ILE:HA	3:A:2112:HOH:O	2.00	0.60
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.83	0.60
1:A:186:ARG:HD2	3:A:2025:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:LYS:HD2	3:C:2321:HOH:O	2.00	0.60
1:A:325:VAL:HG12	1:A:328:ASN:ND2	2.17	0.60
1:A:122:ASP:O	1:A:189:ARG:NH2	2.35	0.59
1:A:56:SER:O	1:A:60:GLU:HG3	2.02	0.59
1:C:274:PHE:HD2	3:C:2139:HOH:O	1.82	0.59
1:C:364:LEU:HD22	1:C:375:PHE:CE1	2.38	0.59
1:B:510:ARG:HB2	1:B:512:THR:HG23	1.84	0.59
1:C:386:ASP:N	1:C:386:ASP:OD2	2.36	0.59
1:A:110:VAL:CG1	1:A:117:ASN:HB3	2.34	0.58
1:A:126:GLU:HG3	3:A:2057:HOH:O	2.03	0.58
1:B:189:ARG:HB3	1:B:189:ARG:HH11	1.68	0.58
1:B:420:CYS:O	1:B:424:SER:HB2	2.04	0.58
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.04	0.58
1:B:476:ASP:HB2	3:B:2170:HOH:O	2.03	0.58
1:C:210:PRO:HG2	1:C:224:SER:HB3	1.85	0.58
1:B:663:HIS:CD2	3:B:2232:HOH:O	2.55	0.57
1:B:325:VAL:HG23	3:B:2120:HOH:O	2.04	0.57
1:C:268:ILE:HG12	1:C:275:HIS:CD2	2.39	0.57
2:F:360:GLN:HG2	2:F:361:ILE:H	1.69	0.57
1:A:110:VAL:HG11	1:A:117:ASN:CB	2.35	0.57
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.86	0.57
1:C:342:LEU:HD12	1:C:376:GLU:HG3	1.87	0.57
1:A:126:GLU:HB3	3:A:2026:HOH:O	2.04	0.56
1:C:191:GLN:NE2	1:C:195:ARG:HH21	2.03	0.56
1:A:225:CYS:CB	3:A:2173:HOH:O	2.52	0.56
1:C:44:ARG:HG3	3:C:2023:HOH:O	2.05	0.56
2:P:3:VAL:CG2	3:P:2003:HOH:O	2.53	0.56
1:B:10:ARG:NH2	1:B:91:LYS:HE2	2.19	0.56
1:C:260:ARG:HD3	3:C:2051:HOH:O	2.06	0.56
1:A:698:ASN:OD1	1:A:733:ASN:ND2	2.36	0.56
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.88	0.56
1:C:294:GLN:HB2	3:C:2155:HOH:O	2.05	0.56
1:C:208:PRO:HB3	3:C:2123:HOH:O	2.06	0.55
1:B:262:ARG:HD3	1:B:274:PHE:CG	2.41	0.55
1:A:651:ILE:HA	3:A:2249:HOH:O	2.05	0.55
1:A:110:VAL:HG11	1:A:117:ASN:HB2	1.89	0.55
1:C:186:ARG:HG2	3:C:2095:HOH:O	2.05	0.55
1:B:207:LEU:HD13	1:B:212:MET:HE1	1.89	0.55
1:A:294:GLN:HB2	1:A:298:ARG:HH11	1.72	0.55
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.88	0.55
1:A:450:ASN:HB2	3:A:2179:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:O	1:C:60:GLU:HG2	2.06	0.54
1:A:10:ARG:HG2	3:A:2006:HOH:O	2.06	0.54
1:A:215:VAL:O	1:A:216:ARG:CB	2.54	0.54
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.89	0.53
1:B:56:SER:O	1:B:60:GLU:HG2	2.08	0.53
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.91	0.53
1:A:195:ARG:HD3	3:A:2083:HOH:O	2.08	0.53
1:A:150:GLN:OE1	1:A:154:LYS:HD2	2.09	0.53
1:B:328:ASN:HB2	3:B:2119:HOH:O	2.07	0.53
1:A:529:LYS:HE3	3:A:2202:HOH:O	2.08	0.52
1:B:11:ASP:CG	1:B:12:GLY:H	2.13	0.52
1:B:647:SER:HB3	1:B:652:LEU:HD13	1.91	0.52
1:A:221:GLN:NE2	1:B:271:GLY:HA3	2.13	0.52
2:P:3:VAL:HG23	3:P:2003:HOH:O	2.08	0.52
1:A:114:LYS:HD2	3:A:2074:HOH:O	2.09	0.52
1:B:621:PRO:HD3	1:B:694:SER:OG	2.08	0.52
1:A:110:VAL:HG13	1:A:117:ASN:HB3	1.91	0.52
1:B:268:ILE:CG2	3:B:2045:HOH:O	2.57	0.52
1:C:294:GLN:HG2	1:C:295:GLY:H	1.75	0.52
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.92	0.52
1:A:207:LEU:HD13	1:A:212:MET:HE3	1.92	0.51
1:C:362:PRO:HA	3:C:2191:HOH:O	2.09	0.51
1:A:290:LYS:HG2	1:A:296:GLY:O	2.10	0.51
1:A:630:ASN:O	1:A:657:PRO:HG3	2.11	0.51
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.92	0.51
1:B:210:PRO:HG2	1:B:224:SER:HB3	1.92	0.51
1:C:585:LYS:HE3	3:C:2280:HOH:O	2.11	0.51
1:A:4:ASN:HA	3:A:2002:HOH:O	2.10	0.51
1:B:207:LEU:HD13	1:B:212:MET:CE	2.41	0.51
1:B:342:LEU:O	1:B:342:LEU:HD12	2.11	0.51
1:A:325:VAL:HG12	1:A:328:ASN:HD21	1.76	0.50
1:C:321:ASN:HA	3:C:2205:HOH:O	2.10	0.50
1:C:553:LYS:O	1:C:557:GLU:HG2	2.11	0.50
1:C:556:ASN:CA	3:C:2291:HOH:O	2.51	0.50
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.92	0.50
1:A:21:LYS:HE3	3:A:2030:HOH:O	2.11	0.49
1:C:447:LYS:HE3	3:C:2233:HOH:O	2.11	0.49
1:C:139:ARG:NH2	1:C:198:ASP:OD1	2.45	0.49
1:A:458:GLU:OE2	1:A:510:ARG:HD2	2.12	0.49
1:C:611:LEU:HA	3:C:2291:HOH:O	2.12	0.49
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:ALA:HB3	3:C:2283:HOH:O	2.11	0.49
1:B:212:MET:HE2	1:B:212:MET:HA	1.93	0.49
1:A:144:SER:O	1:A:147:ALA:HB3	2.13	0.49
1:A:262:ARG:HD2	1:A:274:PHE:CB	2.43	0.49
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.94	0.48
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.47	0.48
1:C:297:VAL:HG13	3:C:2159:HOH:O	2.12	0.48
1:A:58:ILE:O	1:A:62:ILE:HG23	2.12	0.48
1:A:425:PRO:HG3	1:A:615:THR:HG22	1.95	0.48
1:B:349:LYS:HD2	3:B:2129:HOH:O	2.13	0.48
1:C:294:GLN:CG	1:C:295:GLY:N	2.77	0.48
1:C:510:ARG:HB2	1:C:512:THR:HG23	1.95	0.48
1:B:379:TYR:O	1:B:383:GLU:HG3	2.14	0.48
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.96	0.48
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.95	0.48
1:C:472:ILE:HG13	1:C:472:ILE:O	2.13	0.48
1:B:560:LYS:HG2	1:B:609:HIS:CD2	2.49	0.48
1:A:527:HIS:HE1	3:A:2195:HOH:O	1.96	0.48
1:C:138:ASP:O	1:C:141:MET:HB2	2.14	0.47
1:A:181:PHE:O	1:A:189:ARG:HD2	2.15	0.47
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.95	0.47
1:C:242:SER:HB2	1:C:452:VAL:HG13	1.95	0.47
2:D:360:GLN:HG2	2:D:361:ILE:HD13	1.96	0.47
1:A:633:ASN:HB3	3:A:2233:HOH:O	2.15	0.47
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.96	0.47
1:A:6:LEU:HB3	3:A:2003:HOH:O	2.14	0.47
1:B:299:GLY:HA3	3:B:2108:HOH:O	2.14	0.47
1:B:274:PHE:CA	3:B:2097:HOH:O	2.62	0.47
1:B:637:PRO:HG2	1:B:669:LEU:HD12	1.97	0.47
1:C:268:ILE:HG12	1:C:275:HIS:NE2	2.30	0.47
1:B:425:PRO:HG2	1:B:615:THR:HG22	1.96	0.47
1:A:4:ASN:N	3:A:2001:HOH:O	2.47	0.47
1:C:396:VAL:HG23	3:C:2182:HOH:O	2.14	0.47
1:A:321:ASN:O	1:A:329:ARG:NE	2.41	0.46
1:A:648:LYS:N	1:A:648:LYS:HD2	2.31	0.46
1:B:443:ALA:O	1:B:444:LEU:HD23	2.15	0.46
1:B:189:ARG:CG	1:B:189:ARG:HH11	2.29	0.46
1:B:411:ARG:HD2	3:B:2146:HOH:O	2.16	0.46
1:C:639:ARG:HD3	3:C:2314:HOH:O	2.16	0.46
1:C:75:PRO:HD2	3:C:2019:HOH:O	2.16	0.46
1:B:565:CYS:HB3	1:B:612:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:HD2	3:C:2171:HOH:O	2.15	0.46
1:A:225:CYS:HB2	3:A:2109:HOH:O	2.15	0.46
1:A:131:MET:HA	1:A:134:PHE:CD2	2.50	0.46
1:A:568:PHE:CE2	1:A:610:GLY:HA2	2.51	0.46
1:A:268:ILE:HG13	1:A:269:ARG:H	1.81	0.45
1:B:447:LYS:HE2	3:B:2158:HOH:O	2.16	0.45
1:A:268:ILE:HG21	3:A:2043:HOH:O	2.15	0.45
1:A:75:PRO:HD2	3:A:2015:HOH:O	2.17	0.45
1:C:341:LYS:HB2	1:C:722:TYR:OH	2.16	0.45
1:C:369:PHE:CD2	1:C:434:ARG:HD2	2.51	0.45
1:A:9:LYS:HD3	3:A:2006:HOH:O	2.16	0.45
1:B:154:LYS:O	1:B:213:SER:HB3	2.15	0.45
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.99	0.45
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.86	0.45
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.46	0.45
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.32	0.45
1:B:274:PHE:HD1	3:B:2097:HOH:O	1.98	0.45
1:C:342:LEU:C	1:C:342:LEU:HD23	2.37	0.45
2:D:360:GLN:OE1	2:D:360:GLN:N	2.50	0.45
1:C:275:HIS:HE1	3:C:2149:HOH:O	1.99	0.44
1:A:320:LYS:HB2	1:A:320:LYS:HE3	1.70	0.44
1:A:440:LEU:HD12	1:A:728:THR:HB	1.99	0.44
1:B:217:THR:OG1	1:B:219:THR:HG22	2.17	0.44
1:B:640:GLY:HA2	1:B:668:LEU:HD13	1.98	0.44
1:C:72:ARG:HG2	1:C:72:ARG:H	1.57	0.44
1:B:189:ARG:CB	1:B:189:ARG:HH11	2.28	0.44
1:B:322:ASN:HB2	3:B:2122:HOH:O	2.16	0.44
1:B:331:ARG:HD2	3:B:2116:HOH:O	2.17	0.44
1:A:130:GLN:HG2	3:A:2064:HOH:O	2.17	0.44
1:B:45:SER:HB2	1:B:61:THR:HG22	1.99	0.44
1:B:172:LEU:O	1:B:176:VAL:HG23	2.18	0.44
1:B:215:VAL:O	1:B:216:ARG:CB	2.63	0.44
1:A:647:SER:N	3:A:2249:HOH:O	2.50	0.44
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.98	0.44
1:A:584:LYS:NZ	1:A:586:ASP:OD1	2.49	0.43
1:B:223:SER:HA	3:B:2078:HOH:O	2.18	0.43
1:C:433:VAL:HG11	1:C:443:ALA:HB1	2.00	0.43
1:C:151:LEU:HA	1:C:155:TYR:HB2	2.00	0.43
1:C:349:LYS:HD3	1:C:351:GLU:OE2	2.18	0.43
1:B:311:LEU:HA	1:B:355:LEU:HB3	2.01	0.43
1:B:619:LEU:HB2	1:B:693:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLU:CD	1:C:187:GLU:H	2.21	0.43
1:B:225:CYS:HB2	3:B:2152:HOH:O	2.18	0.43
1:C:437:ASN:HB2	3:C:2219:HOH:O	2.18	0.43
1:C:226:VAL:HG12	1:C:461:LEU:CD2	2.46	0.43
1:A:135:ILE:HD11	1:A:174:ILE:HG21	2.01	0.43
1:A:221:GLN:OE1	1:A:250:GLN:HG2	2.19	0.43
1:A:331:ARG:HG2	3:A:2136:HOH:O	2.18	0.43
1:C:37:SER:CB	1:C:40:GLN:HB2	2.47	0.43
1:C:645:LYS:CD	3:C:2321:HOH:O	2.65	0.43
3:A:2107:HOH:O	1:B:273:ALA:HB2	2.18	0.43
1:B:274:PHE:HA	3:B:2097:HOH:O	2.19	0.43
1:B:144:SER:O	1:B:147:ALA:HB3	2.19	0.42
1:B:346:ARG:HD2	1:B:352:ASP:O	2.19	0.42
1:C:261:ILE:HG23	1:C:274:PHE:HE1	1.83	0.42
1:A:473:ASN:ND2	3:A:2182:HOH:O	2.52	0.42
1:C:568:PHE:CE2	1:C:610:GLY:HA2	2.55	0.42
1:B:185:PRO:HB2	1:B:187:GLU:HG2	2.01	0.42
1:B:373:GLU:HA	1:B:376:GLU:HB2	2.01	0.42
1:C:427:ASP:OD2	1:C:575:LYS:NZ	2.51	0.42
1:B:225:CYS:HB2	3:B:2151:HOH:O	2.02	0.42
1:B:621:PRO:HD3	1:B:694:SER:CB	2.49	0.42
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.00	0.42
1:A:319:LEU:HD22	1:A:330:VAL:HG23	2.02	0.42
1:A:609:HIS:HD2	3:P:2001:HOH:O	2.02	0.42
1:C:499:PRO:O	1:C:500:ILE:HG13	2.20	0.42
1:C:258:ALA:HB3	1:C:304:LEU:HD21	2.00	0.42
1:B:275:HIS:CE1	3:B:2099:HOH:O	2.72	0.42
1:C:150:GLN:HE21	1:C:627:GLN:CD	2.22	0.42
1:B:247:TYR:CE2	1:B:500:ILE:HD12	2.55	0.42
1:A:9:LYS:NZ	3:A:2004:HOH:O	2.53	0.41
1:A:710:PRO:HA	2:D:362:ASP:HB3	2.02	0.41
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.02	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.08	0.41
1:B:307:PRO:HA	1:B:338:GLN:HB2	2.02	0.41
1:C:171:PHE:HA	1:C:174:ILE:HG22	2.01	0.41
1:C:259:GLY:HA3	1:C:307:PRO:HD3	2.01	0.41
1:A:331:ARG:HD3	3:A:2050:HOH:O	2.19	0.41
1:B:437:ASN:HB2	3:B:2152:HOH:O	2.19	0.41
1:B:472:ILE:HG13	1:B:472:ILE:O	2.20	0.41
1:A:262:ARG:HD2	1:A:274:PHE:HB3	2.02	0.41
1:A:208:PRO:CG	1:A:211:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:HE2	1:A:212:MET:HA	2.03	0.41
1:A:154:LYS:HE3	3:A:2073:HOH:O	2.21	0.41
1:A:648:LYS:N	1:A:648:LYS:CD	2.84	0.41
1:C:268:ILE:C	1:C:270:GLY:H	2.24	0.41
1:C:640:GLY:HA2	1:C:668:LEU:HD13	2.03	0.41
1:A:409:THR:O	1:A:411:ARG:HG2	2.20	0.41
1:A:658:ASP:OD1	1:A:661:HIS:HD2	2.04	0.41
1:B:520:PHE:HB3	1:B:635:ILE:HA	2.02	0.41
1:B:33:LEU:HB3	1:B:76:ASP:HB3	2.02	0.41
1:C:10:ARG:CG	3:C:2006:HOH:O	2.68	0.41
1:C:323:ARG:HH11	1:C:323:ARG:HB2	1.86	0.41
1:C:364:LEU:HD22	1:C:375:PHE:CD1	2.56	0.41
1:B:560:LYS:HG2	1:B:609:HIS:CG	2.56	0.41
1:B:622:SER:O	1:B:633:ASN:HB3	2.21	0.41
1:C:196:PHE:HZ	1:C:207:LEU:HD11	1.85	0.41
1:C:384:LYS:O	1:C:385:ASP:C	2.59	0.41
1:B:511:ARG:O	1:B:613:ASN:HB3	2.21	0.41
1:A:64:LYS:HE2	1:A:650:GLY:HA3	2.02	0.40
1:C:294:GLN:HG2	1:C:295:GLY:N	2.36	0.40
1:C:434:ARG:NE	3:C:2217:HOH:O	2.53	0.40
1:C:21:LYS:HD3	3:C:2015:HOH:O	2.22	0.40
1:A:98:GLU:HG2	3:A:2017:HOH:O	2.21	0.40
1:C:377:ARG:O	1:C:381:LYS:HB2	2.22	0.40
1:C:54:LYS:HE2	3:C:2007:HOH:O	2.21	0.40
1:A:10:ARG:HB3	3:A:2007:HOH:O	2.21	0.40
1:A:59:HIS:HA	1:A:62:ILE:HD13	2.02	0.40
1:C:144:SER:O	1:C:147:ALA:HB3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2016:HOH:O	3:C:2021:HOH:O[15_554]	1.91	0.29
3:B:2024:HOH:O	3:B:2246:HOH:O[2_665]	1.92	0.28

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	731/761 (96%)	691 (94%)	33 (4%)	7 (1%)	18	43
1	B	731/761 (96%)	692 (95%)	29 (4%)	10 (1%)	13	33
1	C	731/761 (96%)	699 (96%)	24 (3%)	8 (1%)	17	40
2	D	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2236/2363 (95%)	2120 (95%)	91 (4%)	25 (1%)	17	40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	294	GLN
1	A	300	GLY
1	B	15	GLU
1	B	216	ARG
1	C	384	LYS
1	A	5	LEU
1	A	298	ARG
1	A	648	LYS
1	B	294	GLN
1	B	295	GLY
1	C	216	ARG
1	C	272	GLU
1	C	267	PRO
1	C	451	ASP
1	B	11	ASP
1	B	12	GLY
1	B	270	GLY

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Mol	Chain	Res	Type
1	C	12	GLY
1	B	296	GLY
1	C	300	GLY
1	B	300	GLY
1	B	730	TYR
1	C	270	GLY
1	A	295	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	628/650 (97%)	585 (93%)	43 (7%)	18 41
1	B	628/650 (97%)	589 (94%)	39 (6%)	21 46
1	C	628/650 (97%)	591 (94%)	37 (6%)	23 49
2	D	16/19 (84%)	15 (94%)	1 (6%)	21 46
2	E	16/19 (84%)	13 (81%)	3 (19%)	2 5
2	F	16/19 (84%)	13 (81%)	3 (19%)	2 5
2	P	3/19 (16%)	3 (100%)	0	100 100
All	All	1935/2026 (96%)	1809 (94%)	126 (6%)	20 44

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	17	ILE
1	A	21	LYS
1	A	62	ILE
1	A	72	ARG
1	A	96	GLN
1	A	117	ASN
1	A	130	GLN
1	A	141	MET
1	A	149	LYS

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Mol	Chain	Res	Type
1	A	158	GLN
1	A	164	GLU
1	A	189	ARG
1	A	206	SER
1	A	216	ARG
1	A	268	ILE
1	A	269	ARG
1	A	297	VAL
1	A	298	ARG
1	A	317	LEU
1	A	321	ASN
1	A	364	LEU
1	A	381	LYS
1	A	384	LYS
1	A	391	GLN
1	A	393	VAL
1	A	394	LYS
1	A	440	LEU
1	A	447	LYS
1	A	452	VAL
1	A	462	CYS
1	A	463	THR
1	A	474	ASN
1	A	484	LEU
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	645	LYS
1	A	648	LYS
1	A	696	ASN
1	A	708	LYS
1	B	5	LEU
1	B	9	LYS
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	44	ARG
1	B	96	GLN
1	B	98	GLU
1	B	139	ARG

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Mol	Chain	Res	Type
1	B	141	MET
1	B	160	ARG
1	B	161	VAL
1	B	183	ASN
1	B	189	ARG
1	B	262	ARG
1	B	297	VAL
1	B	315	SER
1	B	317	LEU
1	B	320	LYS
1	B	325	VAL
1	B	364	LEU
1	B	366	ASP
1	B	373	GLU
1	B	376	GLU
1	B	389	ARG
1	B	391	GLN
1	B	394	LYS
1	B	396	VAL
1	B	440	LEU
1	B	452	VAL
1	B	462	CYS
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	510	ARG
1	B	616	LEU
1	B	623	GLU
1	B	625	SER
1	B	706	SER
1	C	5	LEU
1	C	6	LEU
1	C	9	LYS
1	C	10	ARG
1	C	13	SER
1	C	55	THR
1	C	72	ARG
1	C	111	GLU
1	C	118	HIS
1	C	139	ARG
1	C	141	MET
1	C	187	GLU

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Mol	Chain	Res	Type
1	C	189	ARG
1	C	206	SER
1	C	207	LEU
1	C	269	ARG
1	C	317	LEU
1	C	320	LYS
1	C	361	VAL
1	C	364	LEU
1	C	381	LYS
1	C	384	LYS
1	C	386	ASP
1	C	404	GLN
1	C	408	SER
1	C	440	LEU
1	C	452	VAL
1	C	462	CYS
1	C	465	SER
1	C	474	ASN
1	C	484	LEU
1	C	557	GLU
1	C	585	LYS
1	C	616	LEU
1	C	625	SER
1	C	626	SER
1	C	708	LYS
2	D	361	ILE
2	E	360	GLN
2	E	361	ILE
2	E	367	THR
2	F	360	GLN
2	F	362	ASP
2	F	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	88	HIS
1	A	183	ASN
1	A	221	GLN
1	A	328	ASN
1	A	609	HIS

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Mol	Chain	Res	Type
1	A	630	ASN
1	A	633	ASN
1	A	661	HIS
1	A	663	HIS
1	B	35	ASN
1	B	130	GLN
1	B	250	GLN
1	B	527	HIS
1	B	630	ASN
1	B	661	HIS
1	B	663	HIS
1	B	696	ASN
1	C	4	ASN
1	C	46	HIS
1	C	59	HIS
1	C	183	ASN
1	C	191	GLN
1	C	250	GLN
1	C	328	ASN
1	C	456	ASN
1	C	630	ASN
1	C	661	HIS
1	C	663	HIS
2	D	360	GLN
2	F	372	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TY2	A	731	1	13,13,14	3.15	3 (23%)	15,17,19	1.90	5 (33%)
1	TY2	B	731	1	13,13,14	3.20	3 (23%)	15,17,19	1.95	3 (20%)
1	TY2	C	731	1	13,13,14	3.07	3 (23%)	15,17,19	2.10	5 (33%)

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
1	TY2	A	731	1	-	0/4/6/8	0/1/1/1
1	TY2	B	731	1	-	0/4/6/8	0/1/1/1
1	TY2	C	731	1	-	0/4/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	TY2	CD2-CE2	-6.83	1.30	1.40
1	B	731	TY2	CD2-CE2	-6.71	1.30	1.40
1	C	731	TY2	CD2-CE2	-6.66	1.30	1.40
1	B	731	TY2	CD2-CG	-4.94	1.30	1.39
1	A	731	TY2	CD2-CG	-4.85	1.30	1.39
1	C	731	TY2	CD2-CG	-4.49	1.31	1.39
1	A	731	TY2	CE2-CZ	7.14	1.50	1.40
1	C	731	TY2	CE2-CZ	7.17	1.50	1.40
1	B	731	TY2	CE2-CZ	7.40	1.50	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	731	TY2	CB-CA-C	-5.25	101.29	111.41
1	B	731	TY2	CB-CA-C	-4.59	102.57	111.41
1	A	731	TY2	CB-CA-C	-4.14	103.43	111.41
1	B	731	TY2	CD1-CE1-CZ	-3.77	116.70	120.51
1	C	731	TY2	CD1-CE1-CZ	-3.39	117.08	120.51
1	A	731	TY2	CD1-CE1-CZ	-3.10	117.38	120.51
1	C	731	TY2	CB-CG-CD2	-2.53	115.82	120.43
1	A	731	TY2	CB-CG-CD2	-2.44	115.97	120.43
1	A	731	TY2	CG-CB-CA	2.10	118.52	114.29
1	C	731	TY2	OH-CZ-CE2	2.28	119.83	116.19
1	A	731	TY2	OH-CZ-CE2	2.56	120.27	116.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	731	TY2	OH-CZ-CE2	2.74	120.56	116.19
1	C	731	TY2	CD1-CG-CD2	2.83	122.57	118.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	733/761 (96%)	0.16	22 (3%) 51 50	21, 37, 64, 86	0
1	B	733/761 (96%)	0.09	15 (2%) 65 66	24, 38, 60, 83	0
1	C	733/761 (96%)	-0.02	8 (1%) 80 81	14, 28, 52, 78	0
2	D	16/20 (80%)	1.53	3 (18%) 1 1	69, 84, 89, 91	0
2	E	16/20 (80%)	1.38	2 (12%) 4 3	72, 84, 89, 90	0
2	F	16/20 (80%)	1.08	2 (12%) 4 3	62, 79, 89, 89	0
2	P	3/20 (15%)	0.72	0 100 100	27, 27, 30, 36	0
All	All	2250/2363 (95%)	0.10	52 (2%) 61 61	14, 35, 66, 91	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	11.0
1	A	271	GLY	7.5
1	B	270	GLY	7.0
1	C	271	GLY	6.8
1	A	737	GLY	5.9
1	B	273	ALA	5.9
1	C	270	GLY	5.7
1	A	270	GLY	4.8
2	D	372	ASN	4.8
1	B	297	VAL	4.7
1	A	296	GLY	4.4
1	C	273	ALA	4.2
1	B	271	GLY	4.0
1	A	274	PHE	3.9
1	B	274	PHE	3.9
2	F	360	GLN	3.7
1	C	274	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.5
2	F	361	ILE	3.4
1	A	13	SER	3.4
1	A	14	THR	3.4
1	A	297	VAL	3.4
1	A	6	LEU	3.3
1	A	268	ILE	3.3
1	C	272	GLU	3.2
1	A	298	ARG	3.2
1	B	12	GLY	3.0
1	C	737	GLY	3.0
2	E	368	ASP	2.9
1	C	296	GLY	2.9
1	A	4	ASN	2.9
1	A	323	ARG	2.8
2	E	372	ASN	2.8
1	A	11	ASP	2.8
1	A	16	ARG	2.7
1	B	296	GLY	2.6
1	C	297	VAL	2.6
1	B	14	THR	2.6
1	B	268	ILE	2.6
1	B	6	LEU	2.4
1	B	161	VAL	2.4
1	A	160	ARG	2.3
1	A	53	ILE	2.3
2	D	373	PHE	2.3
1	A	473	ASN	2.2
1	A	161	VAL	2.2
1	A	17	ILE	2.1
1	B	295	GLY	2.1
2	D	364	GLU	2.1
1	B	8	THR	2.1
1	B	272	GLU	2.0
1	B	10	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TY2	B	731	13/14	0.93	0.17	-	36,39,40,40	0
1	TY2	A	731	13/14	0.95	0.16	-	35,39,40,40	0
1	TY2	C	731	13/14	0.95	0.14	-	27,32,34,34	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.