Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X0X
Title	:	RIBONUCLEOTIDE REDUCTASE R1 SUBUNIT OF E. COLI TO 2.3 A RESOLUTION
Authors	:	Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on	:	2009-12-18
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

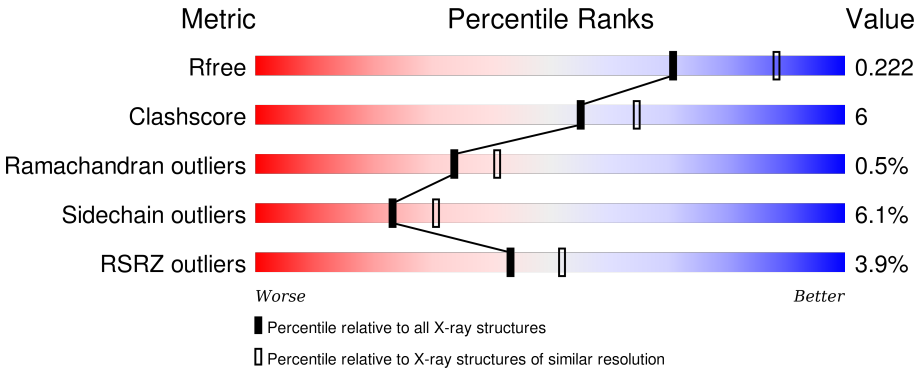
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	4% 80% 13%
1	B	761	3% 81% 12%
1	C	761	2% 82% 11%
2	D	20	20% 70% 10% 20%
2	E	20	25% 70% 5% 5% 20%

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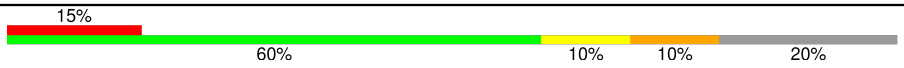
Mol	Chain	Length	Quality of chain
2	F	20	
2	P	20	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1738	-	-	-	X
3	SO4	B	1738	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18869 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.

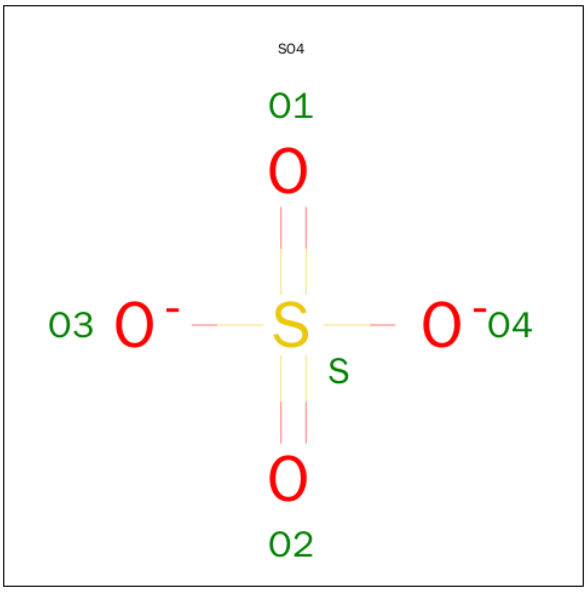
- Molecule 1 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5804	3688	995	1097	24			
1	B	728	Total	C	N	O	S	0	0	0
			5804	3688	995	1097	24			
1	C	728	Total	C	N	O	S	0	0	0
			5804	3688	995	1097	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

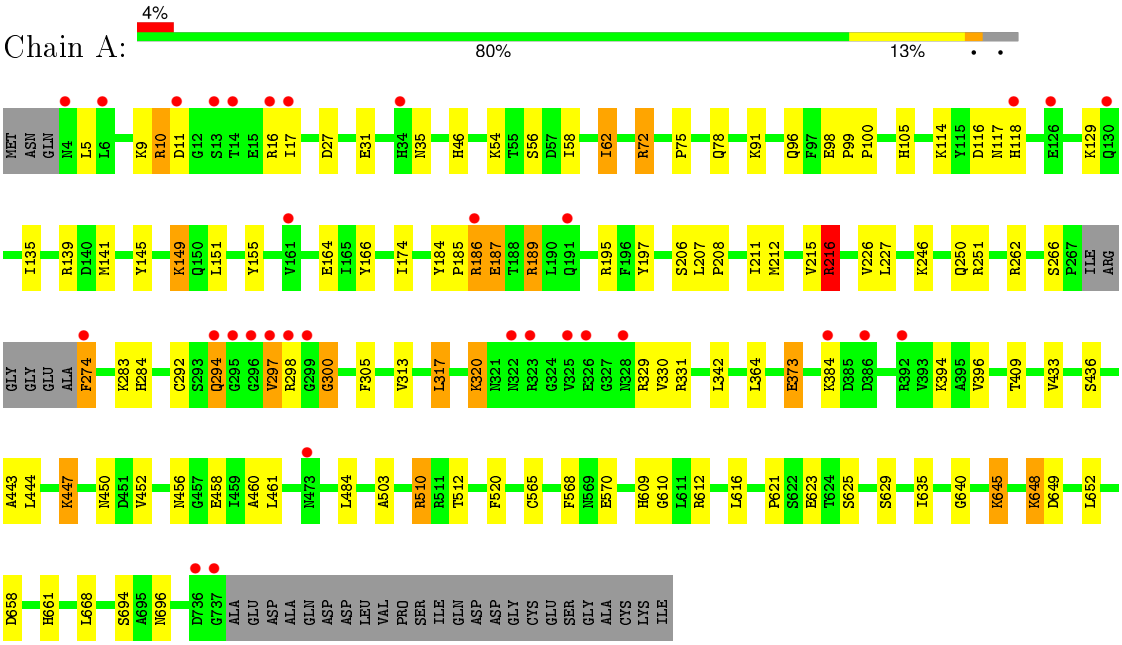
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	304	Total O 304 304	0	0
4	B	306	Total O 306 306	0	0
4	C	411	Total O 411 411	0	0
4	D	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0
4	P	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

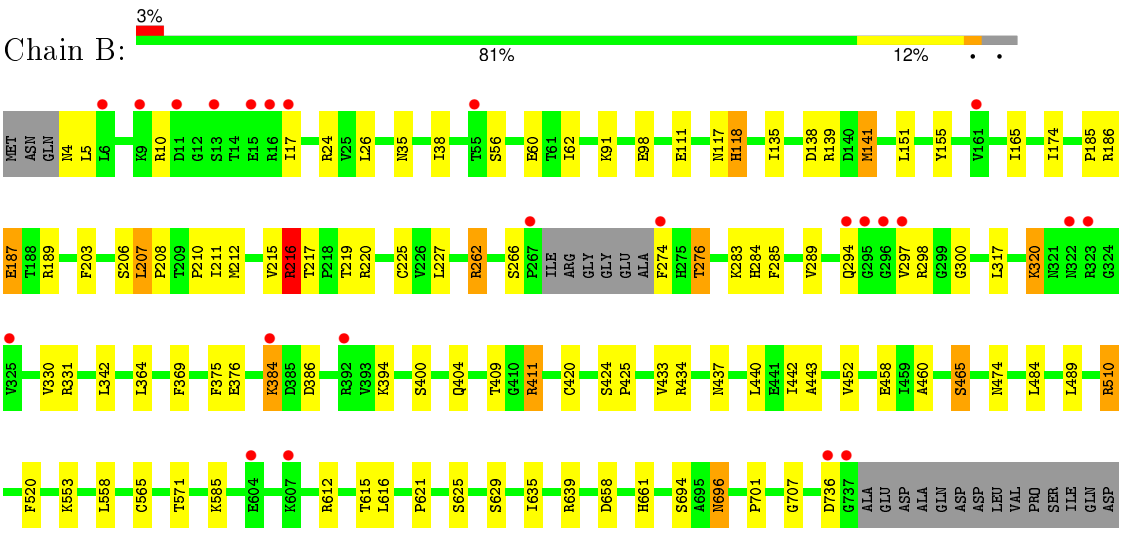
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain A:



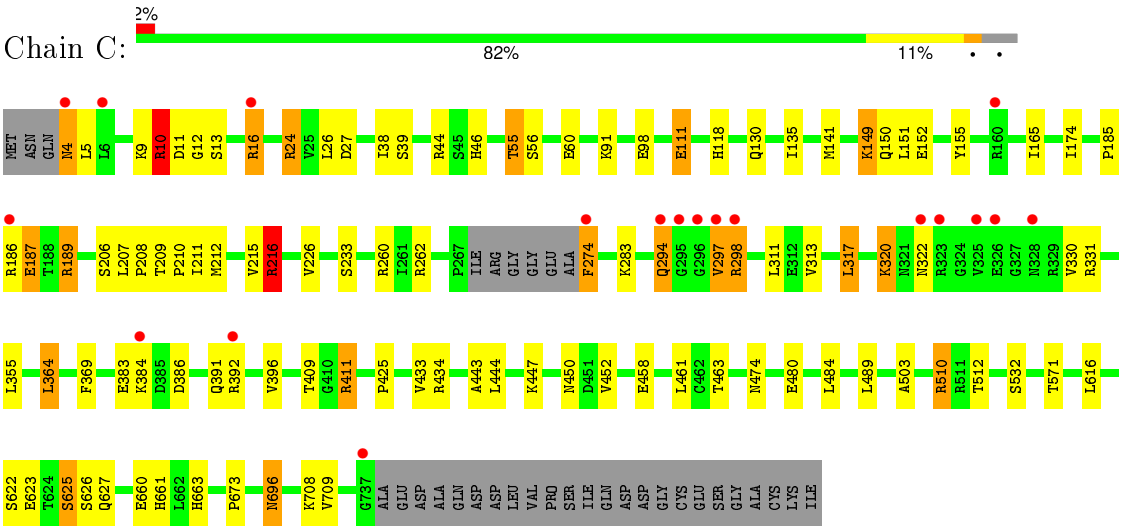
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain B:



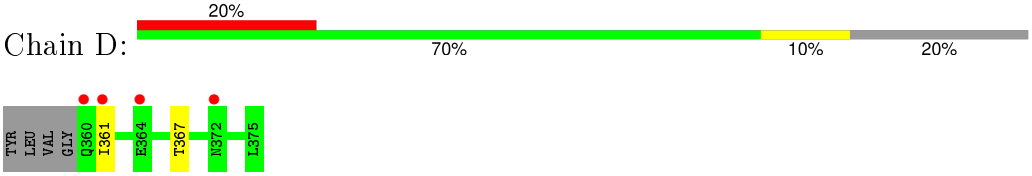
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C:



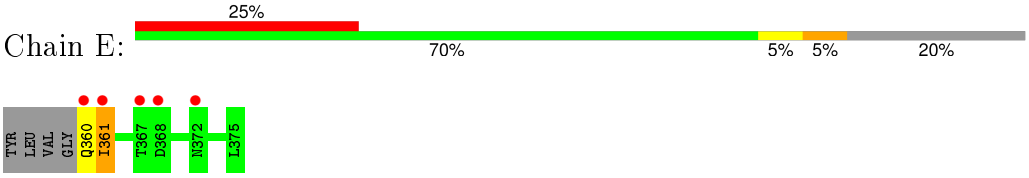
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

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	223.88Å 223.88Å 336.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.30 56.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (169.03-2.30) 100.0 (56.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.224 0.182 , 0.222	Depositor DCC
R_{free} test set	7167 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 142907 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18869	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 2.87% 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: SO4

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	0.53	0/5931	0.64	3/8033 (0.0%)
1	B	0.53	0/5931	0.64	4/8033 (0.0%)
1	C	0.63	0/5931	0.72	7/8033 (0.1%)
2	D	0.50	0/129	0.62	0/173
2	E	0.47	0/129	0.63	0/173
2	F	0.49	0/129	0.62	0/173
2	P	0.68	0/27	0.55	0/36
All	All	0.56	0/18207	0.67	14/24654 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	216	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	C	510	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	C	216	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	216	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	216	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	216	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	510	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	510	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	510	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	216	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	216	ARG	CG-CD-NE	-5.42	100.42	111.80
1	C	364	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	616	LEU	CA-CB-CG	-5.20	103.34	115.30
1	B	510	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	5804	0	5728	82	0
1	B	5804	0	5728	58	0
1	C	5804	0	5728	82	0
2	D	129	0	111	0	0
2	E	129	0	111	1	0
2	F	129	0	111	3	0
2	P	27	0	31	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	304	0	0	18	0
4	B	306	0	0	12	1
4	C	411	0	0	21	1
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	1	0
4	P	1	0	0	2	0
All	All	18869	0	17548	224	1

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 6.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HG	4:A:2133:HOH:O	1.38	1.21
1:C:189:ARG:NH1	4:C:2117:HOH:O	1.87	1.07
1:A:186:ARG:HH11	1:A:186:ARG:HG3	1.25	0.99
1:B:274:PHE:HA	4:B:2117:HOH:O	1.63	0.96
1:C:450:ASN:HB2	4:C:2242:HOH:O	1.67	0.92
2:P:3:VAL:HA	4:P:2001:HOH:O	1.73	0.87
1:C:155:TYR:CD1	4:C:2095:HOH:O	2.28	0.87
1:C:480:GLU:HB3	4:C:2120:HOH:O	1.74	0.85
1:A:262:ARG:CG	1:A:274:PHE:HB2	2.06	0.85
1:C:155:TYR:HD1	4:C:2095:HOH:O	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:HD3	1:B:274:PHE:HB3	1.62	0.82
1:B:56:SER:O	1:B:60:GLU:HG2	1.79	0.81
1:B:215:VAL:O	1:B:216:ARG:HB3	1.81	0.80
1:B:38:ILE:HG12	4:B:2005:HOH:O	1.82	0.80
1:A:10:ARG:H	1:A:10:ARG:HD3	1.46	0.80
1:C:44:ARG:HD3	4:C:2025:HOH:O	1.81	0.79
1:C:262:ARG:HG2	1:C:274:PHE:HB2	1.65	0.79
1:A:212:MET:O	1:A:216:ARG:NH2	2.14	0.79
1:A:450:ASN:HB2	4:A:2175:HOH:O	1.84	0.77
1:C:215:VAL:O	1:C:216:ARG:HB3	1.84	0.77
1:C:298:ARG:HG2	1:C:298:ARG:HH11	1.48	0.77
1:B:185:PRO:HB2	1:B:187:GLU:HG2	1.67	0.76
1:A:9:LYS:HG3	1:A:10:ARG:NH1	2.00	0.76
1:C:262:ARG:CG	1:C:274:PHE:HB2	2.17	0.75
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.69	0.74
1:A:215:VAL:O	1:A:216:ARG:HB3	1.87	0.74
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.71	0.73
1:A:250:GLN:NE2	4:A:2105:HOH:O	2.22	0.73
1:C:189:ARG:NH2	4:C:2116:HOH:O	2.17	0.72
1:C:260:ARG:HH11	1:C:260:ARG:HG2	1.56	0.71
1:C:24:ARG:HH11	1:C:24:ARG:CG	2.03	0.71
1:A:648:LYS:HE2	1:A:648:LYS:H	1.56	0.69
1:A:186:ARG:NH1	1:A:186:ARG:HG3	2.01	0.69
1:C:189:ARG:NE	4:C:2116:HOH:O	2.09	0.68
1:A:262:ARG:HG3	1:A:274:PHE:HB2	1.75	0.67
1:C:262:ARG:HG2	1:C:274:PHE:CB	2.25	0.67
1:C:283:LYS:HG3	1:C:330:VAL:HG22	1.77	0.66
1:C:622:SER:HG	1:C:626:SER:HG	1.44	0.65
1:C:24:ARG:HH11	1:C:24:ARG:HG3	1.61	0.65
1:A:195:ARG:HD3	4:A:2063:HOH:O	1.97	0.65
1:C:450:ASN:CB	4:C:2242:HOH:O	2.36	0.65
1:A:262:ARG:HG2	1:A:274:PHE:HB2	1.78	0.65
1:C:209:THR:HG23	4:C:2095:HOH:O	1.98	0.64
1:A:648:LYS:HD2	1:A:649:ASP:H	1.63	0.63
1:A:54:LYS:HE2	1:A:56:SER:H	1.62	0.63
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.81	0.63
1:B:212:MET:O	1:B:216:ARG:NH2	2.24	0.63
1:A:396:VAL:HG23	4:A:2137:HOH:O	1.99	0.62
1:A:118:HIS:CE1	4:A:2035:HOH:O	2.52	0.62
1:A:292:CYS:HA	1:B:276:THR:HG21	1.80	0.62
1:C:625:SER:OG	3:C:1738:SO4:O4	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HA	1:A:331:ARG:HG2	1.81	0.62
1:C:27:ASP:HA	1:C:38:ILE:HD11	1.80	0.62
1:A:262:ARG:HG2	1:A:274:PHE:CB	2.31	0.60
1:C:396:VAL:HG23	4:C:2197:HOH:O	2.01	0.60
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.82	0.60
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.83	0.59
1:B:24:ARG:HD2	4:B:2004:HOH:O	2.03	0.59
1:A:16:ARG:HG3	4:A:2001:HOH:O	2.03	0.59
1:A:91:LYS:NZ	4:A:2026:HOH:O	2.34	0.58
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.84	0.58
1:C:10:ARG:HB3	1:C:10:ARG:HH11	1.68	0.58
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.09	0.58
1:B:187:GLU:HB2	4:B:2077:HOH:O	2.03	0.58
1:B:639:ARG:HD3	4:B:2260:HOH:O	2.02	0.58
1:A:75:PRO:O	1:A:78:GLN:HB2	2.04	0.58
4:C:2196:HOH:O	2:F:367:THR:HG22	2.02	0.57
1:C:260:ARG:HG2	1:C:260:ARG:NH1	2.19	0.57
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.33	0.57
1:C:189:ARG:HH11	1:C:189:ARG:CG	2.17	0.57
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.85	0.57
1:A:458:GLU:OE2	1:A:510:ARG:HD2	2.04	0.56
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.86	0.56
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.21	0.56
1:C:155:TYR:CZ	1:C:212:MET:HG3	2.41	0.56
1:C:274:PHE:N	1:C:274:PHE:CD2	2.74	0.56
1:C:260:ARG:HH21	1:C:434:ARG:HH22	1.54	0.56
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.88	0.55
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.88	0.55
1:A:300:GLY:HA2	4:A:2106:HOH:O	2.06	0.55
1:C:189:ARG:HH11	1:C:189:ARG:HG2	1.72	0.55
1:A:373:GLU:HG2	4:A:2150:HOH:O	2.06	0.55
1:A:262:ARG:HD3	1:A:266:SER:HB2	1.88	0.55
1:A:409:THR:CG2	4:A:2156:HOH:O	2.54	0.55
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.89	0.55
1:C:24:ARG:HD2	4:C:2008:HOH:O	2.06	0.54
1:A:658:ASP:OD1	1:A:661:HIS:HD2	1.89	0.54
1:A:207:LEU:HD12	1:A:212:MET:HE1	1.90	0.53
1:A:294:GLN:HB2	1:A:298:ARG:HH11	1.73	0.53
2:F:361:ILE:HD11	4:F:2001:HOH:O	2.08	0.53
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.89	0.53
1:A:58:ILE:O	1:A:62:ILE:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:NH1	1:C:24:ARG:CG	2.69	0.53
1:C:458:GLU:OE2	1:C:510:ARG:HD2	2.08	0.52
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.91	0.52
1:B:696:ASN:N	1:B:696:ASN:HD22	2.08	0.52
1:B:283:LYS:HG3	1:B:330:VAL:HG22	1.92	0.52
1:A:447:LYS:HD2	1:A:456:ASN:O	2.10	0.51
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.92	0.51
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.91	0.51
1:C:155:TYR:CE2	1:C:212:MET:SD	3.03	0.51
1:C:709:VAL:O	2:F:361:ILE:HB	2.11	0.51
1:B:117:ASN:HB2	4:B:2043:HOH:O	2.09	0.51
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.46	0.50
1:B:658:ASP:OD1	1:B:661:HIS:HD2	1.95	0.50
1:A:117:ASN:HB2	4:A:2034:HOH:O	2.11	0.50
1:C:409:THR:O	1:C:411:ARG:HG2	2.12	0.50
1:A:186:ARG:NH1	1:A:186:ARG:CG	2.71	0.49
1:C:320:LYS:HA	1:C:331:ARG:HG2	1.95	0.49
1:B:701:PRO:O	1:B:707:GLY:HA2	2.12	0.49
1:C:189:ARG:NH1	1:C:189:ARG:HG2	2.28	0.49
1:B:342:LEU:HD23	1:B:375:PHE:HE2	1.78	0.49
1:C:383:GLU:O	1:C:392:ARG:NH2	2.46	0.49
1:B:420:CYS:O	1:B:424:SER:HB2	2.13	0.49
1:C:320:LYS:HE2	1:C:411:ARG:HB2	1.95	0.48
1:B:207:LEU:HD22	1:B:211:ILE:HG21	1.95	0.48
1:B:10:ARG:NH1	1:B:91:LYS:HD3	2.27	0.48
1:A:409:THR:HG23	4:A:2156:HOH:O	2.14	0.48
1:A:648:LYS:HD2	1:A:649:ASP:N	2.28	0.48
1:C:56:SER:O	1:C:60:GLU:HG2	2.14	0.48
1:C:10:ARG:CZ	1:C:55:THR:HG21	2.43	0.48
1:C:294:GLN:HB3	4:C:2173:HOH:O	2.13	0.48
1:B:404:GLN:HG3	2:E:361:ILE:HD11	1.96	0.48
1:A:164:GLU:HG3	4:A:2028:HOH:O	2.13	0.48
1:A:185:PRO:HB2	1:A:187:GLU:OE2	2.14	0.47
1:A:9:LYS:HG3	1:A:10:ARG:HH11	1.77	0.47
1:C:274:PHE:HB3	4:C:2168:HOH:O	2.14	0.47
1:A:283:LYS:HD3	4:B:2040:HOH:O	2.14	0.47
2:P:2:LEU:O	2:P:3:VAL:C	2.52	0.47
1:B:474:ASN:HB3	4:B:2189:HOH:O	2.13	0.47
1:B:736:ASP:O	1:B:736:ASP:OD1	2.33	0.47
1:C:298:ARG:HG2	1:C:298:ARG:NH1	2.25	0.47
1:C:150:GLN:HE21	1:C:627:GLN:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:CG	1:A:118:HIS:HD2	2.17	0.47
1:C:10:ARG:HB3	1:C:10:ARG:NH1	2.30	0.47
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.97	0.47
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.97	0.47
1:C:298:ARG:CG	1:C:298:ARG:HH11	2.24	0.46
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.96	0.46
1:A:262:ARG:CG	1:A:274:PHE:CB	2.83	0.46
1:B:165:ILE:HD13	4:B:2059:HOH:O	2.15	0.46
1:C:461:LEU:HD11	1:C:503:ALA:HB1	1.97	0.46
1:C:16:ARG:H	1:C:16:ARG:NE	2.13	0.46
1:C:663:HIS:HD2	4:C:2356:HOH:O	1.98	0.46
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.98	0.46
1:A:10:ARG:N	1:A:10:ARG:HD3	2.22	0.46
1:B:384:LYS:HE3	1:B:384:LYS:HA	1.96	0.46
1:A:145:TYR:CZ	1:A:149:LYS:HD3	2.51	0.46
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.98	0.45
1:B:409:THR:O	1:B:411:ARG:HG2	2.16	0.45
1:A:609:HIS:HD2	4:C:2058:HOH:O	1.99	0.45
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.99	0.45
1:B:118:HIS:HB3	4:B:2044:HOH:O	2.17	0.45
1:C:660:GLU:OE2	1:C:661:HIS:NE2	2.50	0.45
1:A:100:PRO:HG2	1:A:105:HIS:HB2	1.99	0.45
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.99	0.45
1:C:212:MET:O	1:C:216:ARG:NH2	2.39	0.45
1:A:568:PHE:CE2	1:A:610:GLY:HA2	2.52	0.45
1:C:149:LYS:HE2	1:C:152:GLU:OE1	2.17	0.45
1:B:285:PHE:O	1:B:289:VAL:HG23	2.17	0.44
1:C:9:LYS:O	1:C:11:ASP:N	2.49	0.44
1:B:26:LEU:HB3	1:B:38:ILE:HG23	2.00	0.44
1:A:184:TYR:O	1:A:189:ARG:HD3	2.18	0.44
1:C:532:SER:HB2	1:C:673:PRO:HD2	2.00	0.44
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.98	0.44
1:B:203:PHE:HB3	1:B:629:SER:HB2	1.98	0.44
1:B:217:THR:OG1	1:B:219:THR:HG22	2.18	0.44
1:A:215:VAL:O	1:A:216:ARG:CB	2.62	0.44
1:C:10:ARG:H	1:C:10:ARG:CD	2.30	0.44
1:A:114:LYS:HE2	1:A:166:TYR:CE2	2.53	0.43
1:A:294:GLN:HB2	1:A:298:ARG:NH1	2.32	0.43
1:A:645:LYS:HD3	1:A:652:LEU:HB2	2.00	0.43
1:C:46:HIS:HB3	4:C:2026:HOH:O	2.17	0.43
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:VAL:CA	4:P:2001:HOH:O	2.50	0.43
1:A:207:LEU:HD12	1:A:212:MET:CE	2.48	0.43
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.01	0.43
1:B:342:LEU:HD23	1:B:375:PHE:CE2	2.53	0.43
1:B:400:SER:O	1:B:404:GLN:HB2	2.19	0.43
1:A:246:LYS:NZ	4:A:2101:HOH:O	2.52	0.43
1:A:621:PRO:HD3	1:A:694:SER:OG	2.19	0.42
1:C:208:PRO:HB2	1:C:210:PRO:HD2	2.00	0.42
1:A:461:LEU:HD11	1:A:503:ALA:HB1	2.01	0.42
1:A:409:THR:HG21	4:A:2156:HOH:O	2.18	0.42
1:A:292:CYS:CA	1:B:276:THR:HG21	2.49	0.42
1:A:139:ARG:NH2	1:A:197:TYR:CE2	2.87	0.42
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.01	0.42
1:B:437:ASN:HB2	4:B:2174:HOH:O	2.19	0.42
1:A:373:GLU:HG2	1:A:373:GLU:H	1.65	0.42
1:C:26:LEU:HB3	1:C:38:ILE:HG12	2.01	0.42
1:C:10:ARG:NH1	1:C:55:THR:HG21	2.35	0.42
1:A:565:CYS:HB3	1:A:612:ARG:O	2.19	0.42
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.83	0.42
1:B:621:PRO:HD3	1:B:694:SER:OG	2.20	0.42
1:B:262:ARG:HG3	1:B:266:SER:HB2	2.02	0.42
1:C:369:PHE:CD2	1:C:434:ARG:HD2	2.54	0.42
1:A:283:LYS:HG3	1:A:330:VAL:HG22	2.01	0.42
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.08	0.42
1:C:708:LYS:HB3	1:C:708:LYS:HE2	1.74	0.42
1:A:450:ASN:HB2	4:A:2182:HOH:O	2.19	0.42
1:B:553:LYS:HE3	4:B:2226:HOH:O	2.20	0.41
1:B:320:LYS:HA	1:B:331:ARG:HG2	2.01	0.41
1:C:98:GLU:HG2	4:C:2054:HOH:O	2.19	0.41
1:B:425:PRO:O	1:B:571:THR:HB	2.21	0.41
1:B:565:CYS:HB3	1:B:612:ARG:O	2.21	0.41
1:C:425:PRO:O	1:C:571:THR:HB	2.21	0.41
1:C:189:ARG:HB3	1:C:189:ARG:HH11	1.85	0.41
1:C:447:LYS:HE3	4:C:2254:HOH:O	2.20	0.41
1:A:72:ARG:HG2	1:A:72:ARG:H	1.52	0.41
1:B:225:CYS:SG	1:B:442:ILE:HG13	2.61	0.41
1:B:208:PRO:HB2	1:B:210:PRO:HD2	2.02	0.41
1:C:111:GLU:CG	2:P:2:LEU:HB2	2.50	0.41
1:C:233:SER:HA	1:C:274:PHE:HZ	1.86	0.41
1:B:118:HIS:HD2	1:B:220:ARG:NH2	2.18	0.41
1:C:696:ASN:N	1:C:696:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:GLU:OE2	1:B:510:ARG:HD2	2.20	0.41
1:B:297:VAL:HG23	1:B:298:ARG:N	2.36	0.40
1:C:4:ASN:HD22	1:C:4:ASN:HA	1.79	0.40
1:B:138:ASP:O	1:B:141:MET:HB2	2.21	0.40
1:A:46:HIS:HE1	4:A:2005:HOH:O	2.04	0.40
1:B:369:PHE:CG	1:B:434:ARG:HG2	2.56	0.40
1:C:185:PRO:HB2	1:C:187:GLU:HG2	2.02	0.40
1:B:425:PRO:HG2	1:B:615:THR:HG22	2.04	0.40
1:C:91:LYS:CG	4:C:2052:HOH:O	2.69	0.40

All (1) 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)
4:B:2006:HOH:O	4:C:2009:HOH:O[15_554]	2.16	0.04

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	724/761 (95%)	699 (96%)	21 (3%)	4 (1%)	30	36
1	B	724/761 (95%)	693 (96%)	28 (4%)	3 (0%)	39	48
1	C	724/761 (95%)	701 (97%)	18 (2%)	5 (1%)	26	31
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	14 (100%)	0	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2215/2363 (94%)	2134 (96%)	69 (3%)	12 (0%)	34	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	B	294	GLN
1	C	294	GLN
1	A	216	ARG
1	B	216	ARG
1	C	10	ARG
1	C	216	ARG
1	B	300	GLY
1	A	300	GLY
1	C	12	GLY
1	A	297	VAL
1	C	297	VAL

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	626/651 (96%)	589 (94%)	37 (6%)	24 32
1	B	626/651 (96%)	592 (95%)	34 (5%)	27 36
1	C	626/651 (96%)	588 (94%)	38 (6%)	23 30
2	D	16/19 (84%)	14 (88%)	2 (12%)	6 6
2	E	16/19 (84%)	14 (88%)	2 (12%)	6 6
2	F	16/19 (84%)	12 (75%)	4 (25%)	1 0
2	P	3/19 (16%)	3 (100%)	0	100 100
All	All	1929/2029 (95%)	1812 (94%)	117 (6%)	23 30

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	ARG
1	A	11	ASP
1	A	17	ILE
1	A	27	ASP
1	A	31	GLU

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Mol	Chain	Res	Type
1	A	35	ASN
1	A	62	ILE
1	A	72	ARG
1	A	96	GLN
1	A	129	LYS
1	A	141	MET
1	A	149	LYS
1	A	186	ARG
1	A	187	GLU
1	A	189	ARG
1	A	206	SER
1	A	226	VAL
1	A	251	ARG
1	A	274	PHE
1	A	297	VAL
1	A	317	LEU
1	A	320	LYS
1	A	364	LEU
1	A	373	GLU
1	A	384	LYS
1	A	394	LYS
1	A	447	LYS
1	A	452	VAL
1	A	484	LEU
1	A	616	LEU
1	A	623	GLU
1	A	625	SER
1	A	629	SER
1	A	645	LYS
1	A	648	LYS
1	A	696	ASN
1	B	4	ASN
1	B	5	LEU
1	B	17	ILE
1	B	35	ASN
1	B	62	ILE
1	B	98	GLU
1	B	111	GLU
1	B	118	HIS
1	B	139	ARG
1	B	141	MET
1	B	186	ARG

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Mol	Chain	Res	Type
1	B	187	GLU
1	B	189	ARG
1	B	206	SER
1	B	207	LEU
1	B	216	ARG
1	B	262	ARG
1	B	276	THR
1	B	317	LEU
1	B	320	LYS
1	B	364	LEU
1	B	376	GLU
1	B	384	LYS
1	B	386	ASP
1	B	394	LYS
1	B	411	ARG
1	B	440	LEU
1	B	452	VAL
1	B	465	SER
1	B	484	LEU
1	B	585	LYS
1	B	616	LEU
1	B	625	SER
1	B	696	ASN
1	C	4	ASN
1	C	5	LEU
1	C	10	ARG
1	C	13	SER
1	C	16	ARG
1	C	24	ARG
1	C	39	SER
1	C	55	THR
1	C	111	GLU
1	C	118	HIS
1	C	130	GLN
1	C	141	MET
1	C	149	LYS
1	C	165	ILE
1	C	186	ARG
1	C	187	GLU
1	C	189	ARG
1	C	206	SER
1	C	207	LEU

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Mol	Chain	Res	Type
1	C	216	ARG
1	C	226	VAL
1	C	274	PHE
1	C	297	VAL
1	C	298	ARG
1	C	317	LEU
1	C	320	LYS
1	C	322	ASN
1	C	364	LEU
1	C	384	LYS
1	C	386	ASP
1	C	391	GLN
1	C	411	ARG
1	C	452	VAL
1	C	474	ASN
1	C	484	LEU
1	C	623	GLU
1	C	625	SER
1	C	696	ASN
2	D	361	ILE
2	D	367	THR
2	E	360	GLN
2	E	361	ILE
2	F	360	GLN
2	F	361	ILE
2	F	367	THR
2	F	374	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	96	GLN
1	A	183	ASN
1	A	250	GLN
1	A	321	ASN
1	A	322	ASN
1	A	328	ASN
1	A	609	HIS
1	A	630	ASN
1	A	661	HIS
1	B	46	HIS

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Mol	Chain	Res	Type
1	B	130	GLN
1	B	150	GLN
1	B	183	ASN
1	B	250	GLN
1	B	328	ASN
1	B	627	GLN
1	B	630	ASN
1	B	661	HIS
1	B	696	ASN
1	B	733	ASN
1	C	4	ASN
1	C	46	HIS
1	C	183	ASN
1	C	250	GLN
1	C	328	ASN
1	C	456	ASN
1	C	630	ASN
1	C	633	ASN
1	C	696	ASN
1	C	733	ASN
2	D	360	GLN
2	E	360	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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1738	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	B	1738	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	C	1738	-	4,4,4	0.15	0	6,6,6	0.26	0

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	SO4	A	1738	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1738	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1738	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1738	SO4	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	728/761 (95%)	0.02	32 (4%) 38 47	22, 36, 58, 89	0
1	B	728/761 (95%)	0.06	24 (3%) 50 59	24, 37, 57, 84	0
1	C	728/761 (95%)	-0.13	19 (2%) 59 68	17, 28, 49, 75	0
2	D	16/20 (80%)	1.07	4 (25%) 1 1	70, 86, 91, 92	0
2	E	16/20 (80%)	1.33	5 (31%) 1 1	69, 85, 91, 92	0
2	F	16/20 (80%)	1.18	3 (18%) 2 2	57, 75, 82, 85	0
2	P	3/20 (15%)	0.80	0 100 100	29, 29, 39, 45	0
All	All	2235/2363 (94%)	0.01	87 (3%) 43 52	17, 34, 63, 92	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	GLY	10.4
1	A	296	GLY	8.4
1	B	297	VAL	8.4
1	A	737	GLY	8.3
1	C	297	VAL	7.7
1	B	274	PHE	7.2
1	C	296	GLY	7.0
1	B	737	GLY	6.8
1	A	297	VAL	6.3
1	A	323	ARG	6.2
1	B	11	ASP	5.8
1	C	295	GLY	5.5
1	B	323	ARG	5.0
1	B	9	LYS	5.0
1	B	295	GLY	4.8
2	E	360	GLN	4.7
1	B	325	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	298	ARG	4.0
1	A	274	PHE	3.9
1	B	384	LYS	3.9
1	B	294	GLN	3.8
1	A	4	ASN	3.7
2	F	360	GLN	3.7
1	C	326	GLU	3.6
1	C	737	GLY	3.5
1	A	299	GLY	3.5
1	C	274	PHE	3.5
1	A	295	GLY	3.5
1	C	294	GLN	3.4
1	A	322	ASN	3.4
1	A	6	LEU	3.3
1	B	736	ASP	3.3
1	B	322	ASN	3.2
1	A	13	SER	3.2
2	D	361	ILE	3.2
2	D	360	GLN	3.2
1	A	17	ILE	3.1
1	C	323	ARG	3.1
2	F	367	THR	3.0
1	C	325	VAL	3.0
1	A	126	GLU	3.0
1	C	298	ARG	2.9
1	A	473	ASN	2.9
1	A	325	VAL	2.9
1	B	161	VAL	2.9
1	C	16	ARG	2.8
1	A	328	ASN	2.8
1	B	13	SER	2.8
1	A	34	HIS	2.7
1	B	17	ILE	2.7
1	B	6	LEU	2.6
2	E	361	ILE	2.6
1	C	4	ASN	2.6
1	A	326	GLU	2.5
1	A	736	ASP	2.5
1	A	186	ARG	2.5
2	E	368	ASP	2.5
1	B	604	GLU	2.5
2	F	361	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	322	ASN	2.4
1	C	186	ARG	2.4
1	B	55	THR	2.4
1	A	191	GLN	2.4
1	B	607	LYS	2.4
1	C	392	ARG	2.4
1	B	15	GLU	2.3
1	A	118	HIS	2.3
1	C	384	LYS	2.3
1	A	161	VAL	2.3
2	D	372	ASN	2.3
1	A	384	LYS	2.2
1	B	267	PRO	2.2
1	A	14	THR	2.2
1	B	392	ARG	2.1
1	A	386	ASP	2.1
1	B	16	ARG	2.1
1	A	130	GLN	2.1
1	C	328	ASN	2.1
2	D	364	GLU	2.1
1	A	294	GLN	2.1
2	E	367	THR	2.1
1	C	6	LEU	2.0
1	A	11	ASP	2.0
1	A	392	ARG	2.0
1	C	160	ARG	2.0
2	E	372	ASN	2.0
1	A	16	ARG	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
3	SO4	A	1738	5/5	0.78	0.24	3.58	106,106,107,107	0
3	SO4	B	1738	5/5	0.77	0.25	2.41	123,124,124,124	0
3	SO4	C	1738	5/5	0.83	0.18	1.43	78,80,80,81	0

6.5 Other polymers (i)

There are no such residues in this entry.