Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:22 PM GMT

PDB ID	:	3R1R
Title	:	RIBONUCLEOTIDE REDUCTASE R1 PROTEIN WITH AMPPNP OCCUPYING THE ACTIVITY SITE FROM ESCHERICHIA COLI
Authors	:	Eriksson, M.; Eklund, H.
Deposited on	:	1997-07-21
Resolution	:	3.00 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:

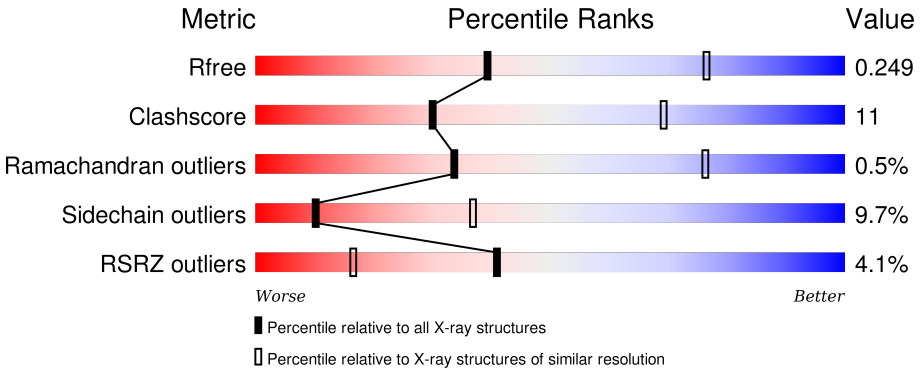
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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% 66% 27%
1	B	761	5% 66% 28%
1	C	761	2% 66% 28%
2	D	20	10% 55% 5% 5% 35%
2	E	20	10% 55% 5% 5% 35%

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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	ATP	A	762	-	-	-	X
3	ATP	B	762	-	-	-	X
3	ATP	C	762	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18027 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.

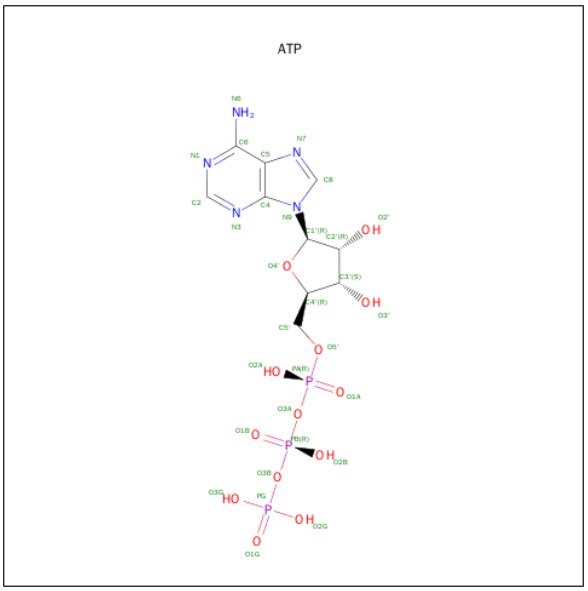
- Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			
1	B	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			
1	C	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	E	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	F	13	Total	C	N	O	0	0	0
			104	62	15	27			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

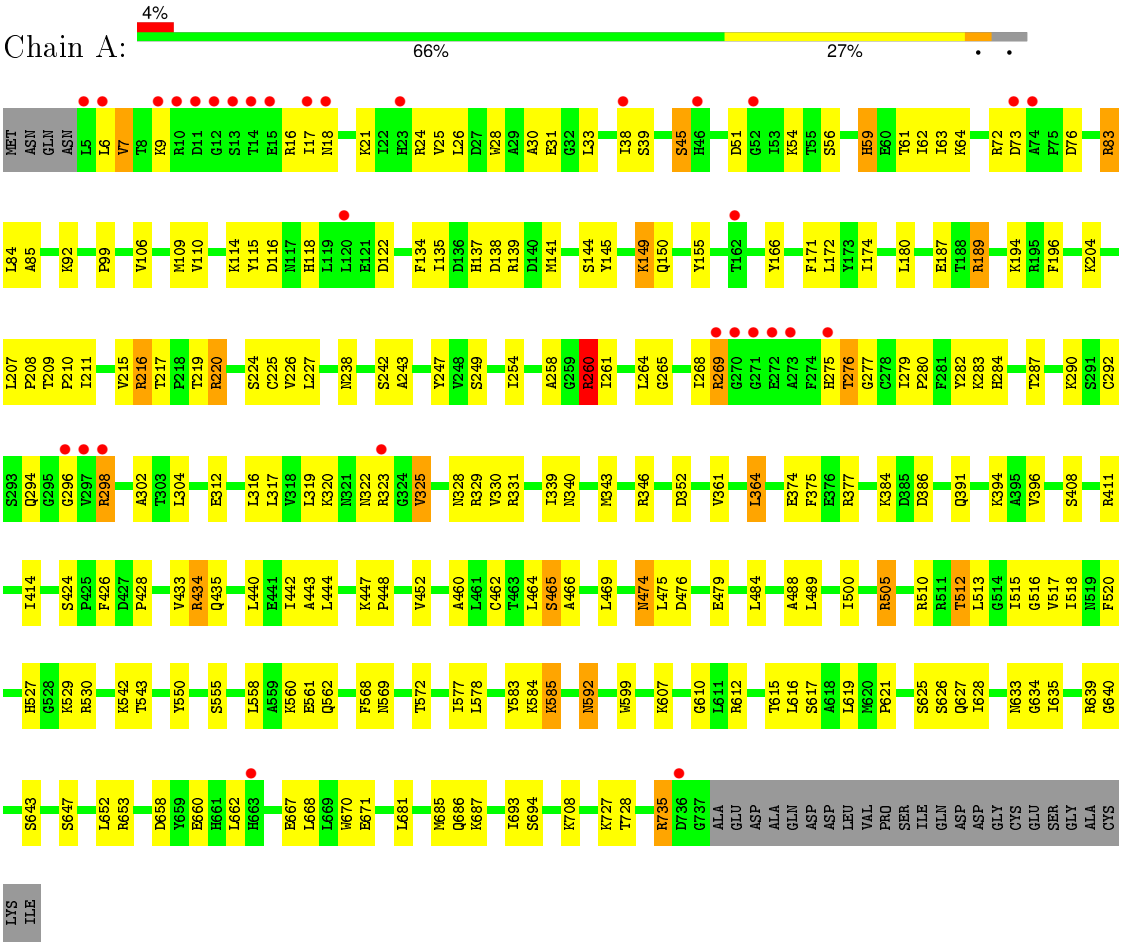
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	28	Total	O	0	0
			28	28		
4	C	29	Total	O	0	0
			29	29		

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.

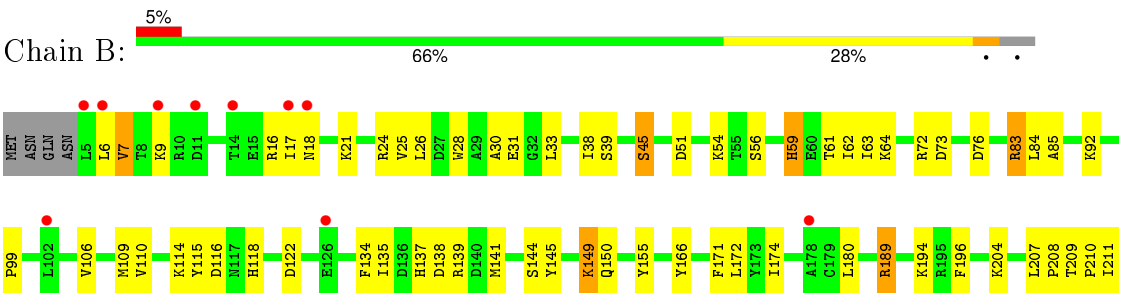
- Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

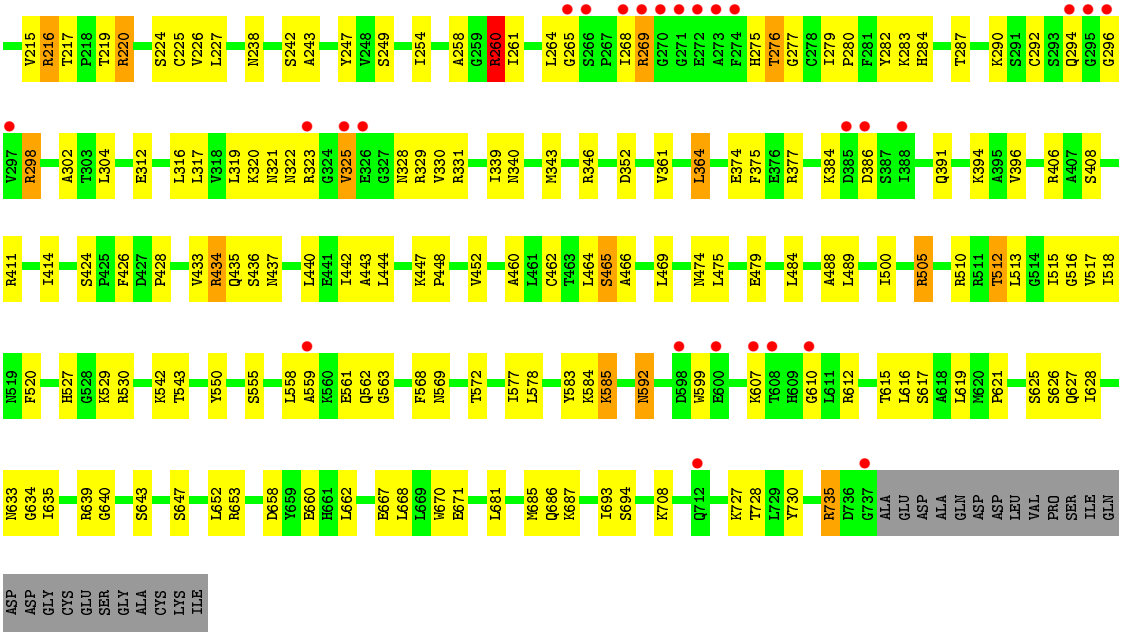
Chain A:



- Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

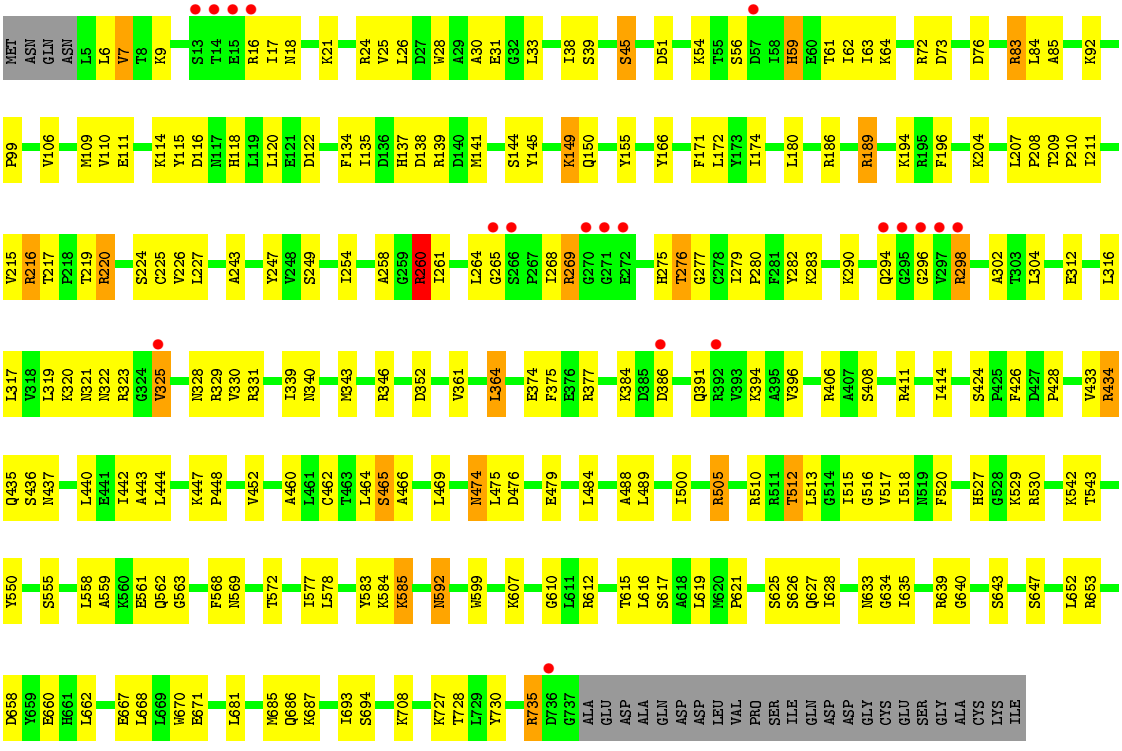
Chain B:





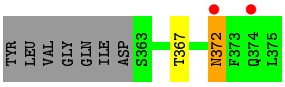
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C:



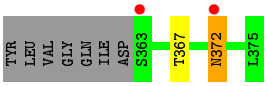
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D:



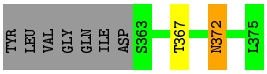
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E:



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F:



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

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	224.61Å 224.61Å 336.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 39.70 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-3.00) 96.0 (39.70-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.263 , 0.287 0.235 , 0.249	Depositor DCC
R_{free} test set	1262 reflections (2.06%)	DCC
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	0 of 63244 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18027	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: ATP

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	0.38	0/5965	0.99	11/8079 (0.1%)
1	B	0.38	0/5965	1.00	11/8079 (0.1%)
1	C	0.38	0/5965	0.99	11/8079 (0.1%)
2	D	0.38	0/104	0.83	0/139
2	E	0.38	0/104	0.83	0/139
2	F	0.38	0/104	0.83	0/139
2	P	0.53	0/27	1.74	1/36 (2.8%)
All	All	0.38	0/18234	0.99	34/24690 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	83	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	C	83	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	434	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	434	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	434	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	C	530	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	530	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	530	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	530	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	530	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	530	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	139	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	139	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	139	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	P	2	LEU	CA-CB-CG	5.73	128.48	115.30
1	B	155	TYR	CB-CG-CD1	5.66	124.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	TYR	CB-CG-CD1	5.65	124.39	121.00
1	C	155	TYR	CB-CG-CD1	5.65	124.39	121.00
1	B	653	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	260	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	260	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	260	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	653	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	653	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	653	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	653	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	653	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	155	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	C	155	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	B	155	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	B	735	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	735	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	735	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5837	0	5762	131	0
1	B	5837	0	5762	132	0
1	C	5837	0	5762	130	0
2	D	104	0	88	3	0
2	E	104	0	88	2	0
2	F	104	0	88	3	0
2	P	27	0	31	4	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
4	A	27	0	0	0	0
4	B	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	29	0	0	0	0
All	All	18027	0	17617	394	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 11.

All (394) 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:B:658:ASP:HB3	1:B:662:LEU:HD12	1.60	0.83
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.60	0.82
1:A:292:CYS:HA	1:B:276:THR:HG21	1.60	0.82
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.60	0.81
1:A:561:GLU:HG2	1:A:562:GLN:HG3	1.65	0.77
1:C:275:HIS:CD2	1:C:277:GLY:H	2.03	0.77
1:B:275:HIS:CD2	1:B:277:GLY:H	2.03	0.77
1:B:561:GLU:HG2	1:B:562:GLN:HG3	1.65	0.77
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.65	0.76
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.68	0.76
1:A:275:HIS:CD2	1:A:277:GLY:H	2.03	0.76
2:D:372:ASN:ND2	2:D:372:ASN:H	1.84	0.75
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.68	0.75
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.68	0.74
1:A:275:HIS:HD2	1:A:277:GLY:H	1.34	0.73
1:C:283:LYS:HG3	1:C:330:VAL:HG22	1.71	0.73
2:E:372:ASN:H	2:E:372:ASN:ND2	1.84	0.73
1:C:275:HIS:HD2	1:C:277:GLY:H	1.34	0.73
1:A:7:VAL:HG23	1:A:17:ILE:HG12	1.71	0.73
1:B:275:HIS:HD2	1:B:277:GLY:H	1.34	0.73
1:A:283:LYS:HG3	1:A:330:VAL:HG22	1.71	0.73
1:B:283:LYS:HG3	1:B:330:VAL:HG22	1.71	0.73
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.71	0.72
2:F:372:ASN:ND2	2:F:372:ASN:H	1.84	0.72
1:B:7:VAL:HG23	1:B:17:ILE:HG12	1.71	0.72
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.25	0.72
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.72	0.71
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.71	0.71
1:C:7:VAL:HG23	1:C:17:ILE:HG12	1.71	0.71
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.72	0.71
1:A:584:LYS:HD2	1:A:585:LYS:HE2	1.72	0.70
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.72	0.70
1:B:584:LYS:HD2	1:B:585:LYS:HE2	1.72	0.70
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.74	0.70
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.74	0.70
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.74	0.70
1:C:584:LYS:HD2	1:C:585:LYS:HE2	1.72	0.70
1:C:26:LEU:HB3	1:C:38:ILE:HD12	1.74	0.69
1:B:215:VAL:O	1:B:216:ARG:HB3	1.92	0.69
1:C:215:VAL:O	1:C:216:ARG:HB3	1.92	0.69
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.74	0.68
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.74	0.68
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.75	0.68
1:A:215:VAL:O	1:A:216:ARG:HB3	1.92	0.68
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.77	0.67
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.77	0.67
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.75	0.66
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.75	0.66
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.77	0.65
1:A:149:LYS:HG2	1:A:652:LEU:HD21	1.79	0.65
1:A:440:LEU:HD12	1:A:728:THR:HB	1.79	0.64
1:C:18:ASN:HD22	1:C:21:LYS:HE3	1.63	0.64
1:B:440:LEU:HD12	1:B:728:THR:HB	1.79	0.64
1:B:18:ASN:HD22	1:B:21:LYS:HE3	1.63	0.64
1:C:440:LEU:HD12	1:C:728:THR:HB	1.79	0.64
1:B:149:LYS:HG2	1:B:652:LEU:HD21	1.79	0.64
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.81	0.63
1:A:18:ASN:HD22	1:A:21:LYS:HE3	1.63	0.63
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.81	0.63
1:C:149:LYS:HG2	1:C:652:LEU:HD21	1.79	0.63
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.81	0.63
1:B:279:ILE:HD13	1:B:319:LEU:HD21	1.80	0.62
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.80	0.62
1:C:111:GLU:OE2	2:P:2:LEU:HB2	2.00	0.62
1:C:279:ILE:HD13	1:C:319:LEU:HD21	1.80	0.61
1:B:30:ALA:HB2	1:B:38:ILE:HD11	1.83	0.61
1:C:30:ALA:HB2	1:C:38:ILE:HD11	1.83	0.61
1:A:30:ALA:HB2	1:A:38:ILE:HD11	1.83	0.60
1:A:276:THR:HG23	1:A:280:PRO:HG2	1.84	0.60
1:A:276:THR:HG21	1:B:292:CYS:HA	1.84	0.59
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.84	0.59
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HG21	1:B:247:TYR:CG	2.38	0.59
1:B:260:ARG:NH2	1:B:434:ARG:HH22	2.00	0.59
1:C:226:VAL:HG21	1:C:247:TYR:CG	2.38	0.59
1:B:196:PHE:HZ	1:B:207:LEU:HD11	1.68	0.59
1:C:276:THR:HG23	1:C:280:PRO:HG2	1.84	0.59
1:C:196:PHE:HZ	1:C:207:LEU:HD11	1.68	0.59
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.85	0.58
1:B:276:THR:HG23	1:B:280:PRO:HG2	1.84	0.58
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.84	0.58
1:A:260:ARG:NH2	1:A:434:ARG:HH22	2.00	0.58
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.38	0.58
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.86	0.58
1:C:325:VAL:HG13	1:C:328:ASN:HB2	1.86	0.58
1:A:196:PHE:HZ	1:A:207:LEU:HD11	1.68	0.58
1:C:260:ARG:NH2	1:C:434:ARG:HH22	2.00	0.58
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.85	0.58
1:C:444:LEU:HD12	1:C:460:ALA:HB1	1.85	0.57
1:C:180:LEU:HD12	1:C:488:ALA:HB1	1.86	0.57
1:A:325:VAL:HG13	1:A:328:ASN:HB2	1.86	0.57
1:B:585:LYS:H	1:B:585:LYS:HD3	1.69	0.57
1:A:180:LEU:HD12	1:A:488:ALA:HB1	1.86	0.57
1:B:180:LEU:HD12	1:B:488:ALA:HB1	1.86	0.57
1:C:585:LYS:HD3	1:C:585:LYS:H	1.69	0.57
1:A:585:LYS:H	1:A:585:LYS:HD3	1.69	0.57
1:A:122:ASP:O	1:A:189:ARG:NH2	2.38	0.57
1:A:145:TYR:CZ	1:A:149:LYS:HD3	2.40	0.56
1:A:442:ILE:HG13	1:A:462:CYS:SG	2.45	0.56
1:B:442:ILE:HG13	1:B:462:CYS:SG	2.45	0.56
1:C:145:TYR:CZ	1:C:149:LYS:HD3	2.40	0.56
1:C:122:ASP:O	1:C:189:ARG:NH2	2.38	0.56
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.88	0.56
1:B:122:ASP:O	1:B:189:ARG:NH2	2.38	0.56
1:C:442:ILE:HG13	1:C:462:CYS:SG	2.45	0.56
1:A:339:ILE:HD12	1:A:414:ILE:HG23	1.88	0.56
1:B:145:TYR:CZ	1:B:149:LYS:HD3	2.40	0.56
1:C:339:ILE:HD12	1:C:414:ILE:HG23	1.88	0.56
1:C:7:VAL:CG2	1:C:17:ILE:HG12	2.36	0.56
1:B:339:ILE:HD12	1:B:414:ILE:HG23	1.88	0.56
1:C:572:THR:HB	1:C:577:ILE:HB	1.88	0.55
1:B:7:VAL:CG2	1:B:17:ILE:HG12	2.36	0.55
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.89	0.55
1:B:572:THR:HB	1:B:577:ILE:HB	1.88	0.55
1:B:254:ILE:O	1:B:302:ALA:HA	2.07	0.55
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.89	0.55
1:A:626:SER:CB	1:A:633:ASN:HD22	2.20	0.55
1:C:215:VAL:O	1:C:216:ARG:CB	2.55	0.55
1:C:254:ILE:O	1:C:302:ALA:HA	2.07	0.55
1:A:215:VAL:O	1:A:216:ARG:CB	2.55	0.54
1:B:215:VAL:O	1:B:216:ARG:CB	2.55	0.54
1:B:626:SER:CB	1:B:633:ASN:HD22	2.20	0.54
1:A:572:THR:HB	1:A:577:ILE:HB	1.88	0.54
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.88	0.54
1:A:59:HIS:O	1:A:63:ILE:HG13	2.07	0.54
1:A:254:ILE:O	1:A:302:ALA:HA	2.07	0.54
1:C:59:HIS:O	1:C:63:ILE:HG13	2.07	0.54
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.89	0.54
1:C:626:SER:CB	1:C:633:ASN:HD22	2.20	0.54
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.88	0.54
1:A:7:VAL:CG2	1:A:17:ILE:HG12	2.36	0.54
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.89	0.53
1:A:462:CYS:HB3	1:A:464:LEU:HD21	1.90	0.53
1:B:59:HIS:O	1:B:63:ILE:HG13	2.07	0.53
1:C:462:CYS:HB3	1:C:464:LEU:HD21	1.91	0.53
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.89	0.53
1:A:226:VAL:HG21	1:A:247:TYR:CD2	2.44	0.53
1:C:217:THR:OG1	1:C:219:THR:HG22	2.10	0.52
1:B:226:VAL:HG21	1:B:247:TYR:CD2	2.44	0.52
1:B:462:CYS:HB3	1:B:464:LEU:HD21	1.90	0.52
1:A:626:SER:HB2	1:A:633:ASN:HD22	1.74	0.52
1:A:217:THR:OG1	1:A:219:THR:HG22	2.10	0.52
1:C:149:LYS:HA	1:C:149:LYS:HE2	1.92	0.52
1:C:322:ASN:HA	1:C:331:ARG:HE	1.74	0.52
1:B:217:THR:OG1	1:B:219:THR:HG22	2.10	0.52
1:B:322:ASN:HA	1:B:331:ARG:HE	1.74	0.52
1:A:569:ASN:H	1:A:569:ASN:ND2	2.08	0.52
1:C:226:VAL:HG21	1:C:247:TYR:CD2	2.44	0.52
1:B:569:ASN:ND2	1:B:569:ASN:H	2.08	0.52
1:B:149:LYS:HA	1:B:149:LYS:HE2	1.92	0.52
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.91	0.52
1:C:569:ASN:ND2	1:C:569:ASN:H	2.08	0.52
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:LEU:HD13	1:C:599:TRP:HE3	1.75	0.52
1:B:578:LEU:HD13	1:B:599:TRP:HE3	1.75	0.52
1:B:518:ILE:HA	1:B:634:GLY:HA2	1.91	0.51
1:A:578:LEU:HD13	1:A:599:TRP:HE3	1.75	0.51
1:A:322:ASN:HA	1:A:331:ARG:HE	1.74	0.51
1:C:59:HIS:CD2	3:C:762:ATP:H4'	2.46	0.51
1:A:621:PRO:HD3	1:A:694:SER:OG	2.10	0.51
1:C:260:ARG:NH2	1:C:434:ARG:NH2	2.59	0.51
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.93	0.51
1:C:626:SER:HB2	1:C:633:ASN:HD22	1.74	0.50
1:B:621:PRO:HD3	1:B:694:SER:OG	2.10	0.50
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.93	0.50
1:B:626:SER:HB2	1:B:633:ASN:HD22	1.74	0.50
1:A:59:HIS:CD2	3:A:762:ATP:H4'	2.46	0.50
1:A:518:ILE:HA	1:A:634:GLY:HA2	1.91	0.50
1:B:18:ASN:HB2	1:B:21:LYS:HE3	1.94	0.50
1:B:260:ARG:NH2	1:B:434:ARG:NH2	2.59	0.50
1:A:260:ARG:NH2	1:A:434:ARG:NH2	2.59	0.50
1:C:18:ASN:HB2	1:C:21:LYS:HE3	1.94	0.50
1:C:621:PRO:HD3	1:C:694:SER:OG	2.10	0.50
1:A:686:GLN:CD	1:A:727:LYS:HD2	2.32	0.50
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.32	0.50
1:B:59:HIS:CD2	3:B:762:ATP:H4'	2.46	0.50
1:C:447:LYS:HZ3	1:C:505:ARG:HH22	1.59	0.49
1:A:447:LYS:HZ3	1:A:505:ARG:HH22	1.60	0.49
1:B:670:TRP:CE2	1:B:735:ARG:HG3	2.48	0.49
1:C:670:TRP:CE2	1:C:735:ARG:HG3	2.48	0.49
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.93	0.49
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.94	0.49
1:B:447:LYS:HZ2	1:B:505:ARG:NH2	2.10	0.49
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.94	0.49
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.32	0.49
1:A:18:ASN:HB2	1:A:21:LYS:HE3	1.94	0.49
1:C:264:LEU:HD12	1:C:265:GLY:N	2.28	0.48
2:F:372:ASN:N	2:F:372:ASN:ND2	2.59	0.48
1:A:670:TRP:CE2	1:A:735:ARG:HG3	2.48	0.48
1:A:264:LEU:HD12	1:A:265:GLY:N	2.28	0.48
1:B:264:LEU:HD12	1:B:265:GLY:N	2.28	0.48
1:A:284:HIS:HA	1:B:287:THR:OG1	2.13	0.48
1:B:592:ASN:HD22	1:B:592:ASN:C	2.17	0.48
1:A:592:ASN:HD22	1:A:592:ASN:C	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASN:C	1:C:592:ASN:HD22	2.17	0.48
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.94	0.48
1:B:583:TYR:CG	1:B:687:LYS:HG3	2.49	0.48
1:A:238:ASN:HB3	1:B:242:SER:OG	2.13	0.48
1:B:116:ASP:OD2	1:B:220:ARG:NH2	2.47	0.48
1:B:681:LEU:O	1:B:685:MET:HG3	2.14	0.48
1:A:242:SER:OG	1:B:238:ASN:HB3	2.13	0.48
1:A:583:TYR:CG	1:A:687:LYS:HG3	2.49	0.48
1:A:106:VAL:O	1:A:110:VAL:HG23	2.14	0.47
1:A:447:LYS:NZ	1:A:505:ARG:NH2	2.63	0.47
1:C:322:ASN:O	1:C:331:ARG:NH2	2.47	0.47
1:C:447:LYS:NZ	1:C:505:ARG:NH2	2.63	0.47
1:C:106:VAL:O	1:C:110:VAL:HG23	2.14	0.47
1:C:681:LEU:O	1:C:685:MET:HG3	2.14	0.47
1:B:447:LYS:NZ	1:B:505:ARG:NH2	2.63	0.47
2:D:372:ASN:HD22	2:D:372:ASN:H	1.61	0.47
1:A:180:LEU:CD1	1:A:488:ALA:HB1	2.44	0.47
1:A:322:ASN:O	1:A:331:ARG:NH2	2.47	0.47
1:C:116:ASP:OD2	1:C:220:ARG:NH2	2.47	0.47
1:A:116:ASP:OD2	1:A:220:ARG:NH2	2.47	0.47
1:B:106:VAL:O	1:B:110:VAL:HG23	2.14	0.47
2:E:372:ASN:H	2:E:372:ASN:HD22	1.61	0.47
2:F:372:ASN:HD22	2:F:372:ASN:H	1.61	0.47
1:C:62:ILE:HD11	1:C:84:LEU:HD22	1.97	0.47
1:B:322:ASN:O	1:B:331:ARG:NH2	2.47	0.47
1:C:583:TYR:CG	1:C:687:LYS:HG3	2.49	0.47
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.50	0.47
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.50	0.47
1:C:294:GLN:HB2	1:C:298:ARG:HG3	1.97	0.47
1:A:681:LEU:O	1:A:685:MET:HG3	2.14	0.47
1:A:150:GLN:HE21	1:A:627:GLN:CD	2.18	0.47
1:A:62:ILE:HD11	1:A:84:LEU:HD22	1.96	0.47
1:B:294:GLN:HB2	1:B:298:ARG:HG3	1.97	0.47
1:B:180:LEU:CD1	1:B:488:ALA:HB1	2.44	0.46
2:D:372:ASN:ND2	2:D:372:ASN:N	2.59	0.46
1:B:258:ALA:HB1	1:B:261:ILE:HD12	1.98	0.46
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.43	0.46
1:C:180:LEU:CD1	1:C:488:ALA:HB1	2.44	0.46
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.43	0.46
1:C:258:ALA:HB1	1:C:261:ILE:HD12	1.98	0.46
1:C:150:GLN:HE21	1:C:627:GLN:CD	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:NH1	1:B:448:PRO:HG3	2.31	0.46
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.43	0.46
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.98	0.46
1:A:512:THR:HG22	1:A:615:THR:HG23	1.97	0.46
1:A:260:ARG:NH1	1:A:448:PRO:HG3	2.31	0.46
1:C:260:ARG:NH1	1:C:448:PRO:HG3	2.31	0.46
1:C:640:GLY:HA2	1:C:668:LEU:HD13	1.98	0.46
1:B:62:ILE:HD11	1:B:84:LEU:HD22	1.97	0.45
1:B:150:GLN:HE21	1:B:627:GLN:CD	2.18	0.45
1:C:512:THR:HG22	1:C:615:THR:HG23	1.97	0.45
1:A:187:GLU:OE2	1:C:186:ARG:HD2	2.16	0.45
1:A:220:ARG:HA	1:A:220:ARG:HD3	1.74	0.45
1:A:294:GLN:HB2	1:A:298:ARG:HG3	1.97	0.45
1:A:268:ILE:O	1:A:269:ARG:HB3	2.16	0.45
1:B:640:GLY:HA2	1:B:668:LEU:HD13	1.98	0.45
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.50	0.45
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.99	0.45
1:A:138:ASP:O	1:A:141:MET:HB2	2.17	0.45
1:B:243:ALA:HA	1:B:500:ILE:HD11	1.99	0.45
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.99	0.45
1:B:268:ILE:O	1:B:269:ARG:HB3	2.16	0.45
1:C:243:ALA:HA	1:C:500:ILE:HD11	1.99	0.45
1:A:209:THR:N	1:A:210:PRO:HD2	2.32	0.45
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.99	0.45
1:C:138:ASP:O	1:C:141:MET:HB2	2.17	0.45
1:B:209:THR:N	1:B:210:PRO:HD2	2.32	0.45
1:B:512:THR:HG22	1:B:615:THR:HG23	1.97	0.45
1:C:268:ILE:O	1:C:269:ARG:HB3	2.16	0.44
1:A:144:SER:O	1:A:145:TYR:C	2.56	0.44
1:A:560:LYS:HA	2:P:1:TYR:N	2.31	0.44
1:B:138:ASP:O	1:B:141:MET:HB2	2.17	0.44
1:C:209:THR:N	1:C:210:PRO:HD2	2.32	0.44
1:C:447:LYS:NZ	1:C:505:ARG:HH22	2.15	0.44
1:A:447:LYS:NZ	1:A:505:ARG:HH22	2.15	0.44
1:B:475:LEU:HD21	1:B:543:THR:HG23	2.00	0.44
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.98	0.44
1:C:520:PHE:HB3	1:C:635:ILE:HA	2.00	0.44
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.53	0.44
1:C:312:GLU:O	1:C:316:LEU:HG	2.18	0.44
1:A:469:LEU:HD11	1:A:517:VAL:HG11	2.00	0.44
1:C:475:LEU:HD21	1:C:543:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:SER:HB3	1:C:61:THR:HG22	1.99	0.44
1:B:312:GLU:O	1:B:316:LEU:HG	2.18	0.44
1:B:275:HIS:HD2	1:B:277:GLY:N	2.10	0.44
1:B:144:SER:O	1:B:145:TYR:C	2.56	0.44
1:B:527:HIS:O	1:B:529:LYS:HE2	2.18	0.44
1:C:527:HIS:O	1:C:529:LYS:HE2	2.18	0.44
1:A:527:HIS:O	1:A:529:LYS:HE2	2.18	0.43
1:B:321:ASN:O	1:B:329:ARG:NE	2.51	0.43
1:B:447:LYS:NZ	1:B:505:ARG:HH22	2.15	0.43
1:A:171:PHE:O	1:A:174:ILE:HG22	2.18	0.43
1:A:475:LEU:HD21	1:A:543:THR:HG23	2.00	0.43
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.53	0.43
1:A:243:ALA:HA	1:A:500:ILE:HD11	1.99	0.43
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.53	0.43
1:C:30:ALA:O	1:C:31:GLU:C	2.56	0.43
1:A:30:ALA:O	1:A:31:GLU:C	2.56	0.43
1:A:287:THR:OG1	1:B:284:HIS:HA	2.18	0.43
1:A:45:SER:HB3	1:A:61:THR:HG22	1.99	0.43
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.99	0.43
1:B:30:ALA:O	1:B:31:GLU:C	2.56	0.43
1:A:619:LEU:HB2	1:A:693:ILE:HG12	2.00	0.43
1:A:329:ARG:HG3	1:A:331:ARG:NH2	2.34	0.43
1:B:171:PHE:O	1:B:174:ILE:HG22	2.18	0.43
1:A:312:GLU:O	1:A:316:LEU:HG	2.18	0.43
1:A:320:LYS:HE2	1:A:411:ARG:HB2	2.01	0.43
1:B:619:LEU:HB2	1:B:693:ILE:HG12	2.00	0.43
1:A:63:ILE:HD13	1:A:85:ALA:HA	2.01	0.43
1:C:321:ASN:O	1:C:329:ARG:NE	2.51	0.43
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.54	0.43
1:B:320:LYS:HE2	1:B:411:ARG:HB2	2.01	0.43
1:C:489:LEU:HB3	1:C:513:LEU:HD22	2.01	0.43
1:B:63:ILE:HD13	1:B:85:ALA:HA	2.01	0.43
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.99	0.43
1:C:619:LEU:HB2	1:C:693:ILE:HG12	2.00	0.42
1:C:144:SER:O	1:C:145:TYR:C	2.56	0.42
1:C:220:ARG:HD3	1:C:220:ARG:HA	1.74	0.42
1:C:320:LYS:HE2	1:C:411:ARG:HB2	2.01	0.42
1:C:469:LEU:HD11	1:C:517:VAL:HG11	2.00	0.42
1:C:282:TYR:CE2	1:C:316:LEU:HD22	2.55	0.42
1:B:45:SER:HB3	1:B:61:THR:HG22	1.99	0.42
1:C:515:ILE:O	1:C:617:SER:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LEU:HD11	1:B:517:VAL:HG11	2.00	0.42
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.54	0.42
1:B:109:MET:HB2	1:B:115:TYR:CD2	2.54	0.42
1:C:171:PHE:O	1:C:174:ILE:HG22	2.19	0.42
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.54	0.42
1:A:364:LEU:HD22	1:A:375:PHE:CD1	2.55	0.42
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.54	0.42
1:C:109:MET:HB2	1:C:115:TYR:CD2	2.54	0.42
1:C:329:ARG:HG3	1:C:331:ARG:NH2	2.34	0.42
1:C:364:LEU:HD22	1:C:375:PHE:CD1	2.55	0.42
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.55	0.42
1:A:282:TYR:CE2	1:A:316:LEU:HD22	2.55	0.42
1:A:346:ARG:HD2	1:A:352:ASP:O	2.20	0.42
1:A:114:LYS:HE2	1:A:166:TYR:CE2	2.55	0.42
1:A:489:LEU:HB3	1:A:513:LEU:HD22	2.01	0.42
1:B:282:TYR:CE2	1:B:316:LEU:HD22	2.55	0.42
1:C:339:ILE:HG23	1:C:343:MET:HB2	2.02	0.42
1:B:339:ILE:HG23	1:B:343:MET:HB2	2.02	0.42
1:C:63:ILE:HD13	1:C:85:ALA:HA	2.01	0.42
1:B:329:ARG:HG3	1:B:331:ARG:NH2	2.34	0.42
1:B:220:ARG:HA	1:B:220:ARG:HD3	1.73	0.41
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.55	0.41
1:A:426:PHE:O	1:A:428:PRO:HD3	2.21	0.41
1:A:339:ILE:HG23	1:A:343:MET:HB2	2.02	0.41
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.55	0.41
1:A:668:LEU:HB2	1:A:671:GLU:HG3	2.01	0.41
1:B:489:LEU:HB3	1:B:513:LEU:HD22	2.01	0.41
1:B:28:TRP:O	1:B:31:GLU:HB2	2.20	0.41
1:B:114:LYS:HE2	1:B:166:TYR:CE2	2.55	0.41
1:C:426:PHE:O	1:C:428:PRO:HD3	2.21	0.41
1:B:364:LEU:HD22	1:B:375:PHE:CD1	2.55	0.41
1:A:466:ALA:HA	1:A:516:GLY:O	2.21	0.41
1:C:21:LYS:O	1:C:25:VAL:HG23	2.21	0.41
1:A:21:LYS:O	1:A:25:VAL:HG23	2.21	0.41
1:B:374:GLU:OE2	1:B:377:ARG:NH2	2.53	0.41
1:C:406:ARG:NH2	1:C:730:TYR:O	2.52	0.41
1:B:26:LEU:HD21	1:B:62:ILE:HD12	2.02	0.41
1:C:172:LEU:HD12	1:C:216:ARG:NH2	2.35	0.41
1:B:466:ALA:HA	1:B:516:GLY:O	2.21	0.41
1:A:374:GLU:OE2	1:A:377:ARG:NH2	2.53	0.41
1:C:114:LYS:HE2	1:C:166:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:O	1:A:617:SER:HA	2.20	0.41
1:C:28:TRP:O	1:C:31:GLU:HB2	2.20	0.41
1:B:339:ILE:HG22	1:B:340:ASN:N	2.36	0.41
1:B:668:LEU:HB2	1:B:671:GLU:HG3	2.01	0.41
1:B:515:ILE:O	1:B:617:SER:HA	2.20	0.41
1:C:275:HIS:HD2	1:C:277:GLY:N	2.10	0.41
1:A:172:LEU:HD12	1:A:216:ARG:NH2	2.35	0.41
1:B:559:ALA:O	1:B:563:GLY:N	2.43	0.41
1:C:374:GLU:OE2	1:C:377:ARG:NH2	2.53	0.41
1:C:26:LEU:HD21	1:C:62:ILE:HD12	2.03	0.41
1:A:18:ASN:HB2	1:A:21:LYS:HD2	2.03	0.41
1:C:668:LEU:HB2	1:C:671:GLU:HG3	2.01	0.41
1:C:346:ARG:HD2	1:C:352:ASP:O	2.20	0.41
1:C:466:ALA:HA	1:C:516:GLY:O	2.21	0.41
1:C:474:ASN:OD1	1:C:476:ASP:HB2	2.21	0.41
1:B:172:LEU:HD12	1:B:216:ARG:NH2	2.35	0.41
1:A:28:TRP:O	1:A:31:GLU:HB2	2.20	0.40
1:B:21:LYS:O	1:B:25:VAL:HG23	2.21	0.40
1:B:426:PHE:O	1:B:428:PRO:HD3	2.21	0.40
1:C:559:ALA:O	1:C:563:GLY:N	2.43	0.40
1:B:436:SER:OG	1:B:437:ASN:N	2.52	0.40
1:A:474:ASN:OD1	1:A:476:ASP:HB2	2.21	0.40
1:B:406:ARG:NH2	1:B:730:TYR:O	2.52	0.40
1:A:568:PHE:CZ	1:A:610:GLY:HA2	2.56	0.40
1:B:346:ARG:HD2	1:B:352:ASP:O	2.20	0.40
1:A:26:LEU:HD21	1:A:62:ILE:HD12	2.02	0.40
1:A:339:ILE:HG22	1:A:340:ASN:N	2.36	0.40
1:C:339:ILE:HG22	1:C:340:ASN:N	2.36	0.40
1:C:568:PHE:CZ	1:C:610:GLY:HA2	2.56	0.40
1:C:436:SER:OG	1:C:437:ASN:N	2.53	0.40
1:B:568:PHE:CZ	1:B:610:GLY:HA2	2.56	0.40
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.51	0.40
1:B:18:ASN:HB2	1:B:21:LYS:CD	2.52	0.40
1:A:18:ASN:HB2	1:A:21:LYS:CD	2.52	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	731/761 (96%)	668 (91%)	59 (8%)	4 (0%)	34	76
1	B	731/761 (96%)	668 (91%)	59 (8%)	4 (0%)	34	76
1	C	731/761 (96%)	668 (91%)	59 (8%)	4 (0%)	34	76
2	D	11/20 (55%)	11 (100%)	0	0	100	100
2	E	11/20 (55%)	11 (100%)	0	0	100	100
2	F	11/20 (55%)	11 (100%)	0	0	100	100
2	P	1/20 (5%)	0	1 (100%)	0	100	100
All	All	2227/2363 (94%)	2037 (92%)	178 (8%)	12 (0%)	34	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ARG
1	B	298	ARG
1	C	298	ARG
1	A	6	LEU
1	A	216	ARG
1	B	6	LEU
1	B	216	ARG
1	C	6	LEU
1	C	216	ARG
1	A	296	GLY
1	B	296	GLY
1	C	296	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	628/651 (96%)	568 (90%)	60 (10%)	10 38
1	B	628/651 (96%)	568 (90%)	60 (10%)	10 38
1	C	628/651 (96%)	568 (90%)	60 (10%)	10 38
2	D	13/19 (68%)	11 (85%)	2 (15%)	3 16
2	E	13/19 (68%)	11 (85%)	2 (15%)	3 16
2	F	13/19 (68%)	11 (85%)	2 (15%)	3 16
2	P	3/19 (16%)	2 (67%)	1 (33%)	0 1
All	All	1926/2029 (95%)	1739 (90%)	187 (10%)	10 37

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	LYS
1	A	16	ARG
1	A	24	ARG
1	A	39	SER
1	A	45	SER
1	A	51	ASP
1	A	54	LYS
1	A	56	SER
1	A	59	HIS
1	A	64	LYS
1	A	72	ARG
1	A	73	ASP
1	A	92	LYS
1	A	118	HIS
1	A	149	LYS
1	A	189	ARG
1	A	204	LYS
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	249	SER
1	A	260	ARG
1	A	269	ARG
1	A	276	THR
1	A	290	LYS

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Mol	Chain	Res	Type
1	A	317	LEU
1	A	323	ARG
1	A	325	VAL
1	A	361	VAL
1	A	364	LEU
1	A	384	LYS
1	A	386	ASP
1	A	391	GLN
1	A	394	LYS
1	A	396	VAL
1	A	408	SER
1	A	424	SER
1	A	435	GLN
1	A	452	VAL
1	A	465	SER
1	A	474	ASN
1	A	484	LEU
1	A	505	ARG
1	A	510	ARG
1	A	512	THR
1	A	542	LYS
1	A	555	SER
1	A	585	LYS
1	A	592	ASN
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	628	ILE
1	A	639	ARG
1	A	643	SER
1	A	647	SER
1	A	660	GLU
1	A	667	GLU
1	A	708	LYS
2	D	367	THR
2	D	372	ASN
1	B	7	VAL
1	B	9	LYS
1	B	16	ARG
1	B	24	ARG
1	B	39	SER
1	B	45	SER

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Mol	Chain	Res	Type
1	B	51	ASP
1	B	54	LYS
1	B	56	SER
1	B	59	HIS
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	92	LYS
1	B	118	HIS
1	B	149	LYS
1	B	189	ARG
1	B	204	LYS
1	B	220	ARG
1	B	224	SER
1	B	225	CYS
1	B	249	SER
1	B	260	ARG
1	B	269	ARG
1	B	276	THR
1	B	290	LYS
1	B	317	LEU
1	B	323	ARG
1	B	325	VAL
1	B	361	VAL
1	B	364	LEU
1	B	384	LYS
1	B	386	ASP
1	B	391	GLN
1	B	394	LYS
1	B	396	VAL
1	B	408	SER
1	B	424	SER
1	B	435	GLN
1	B	452	VAL
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	505	ARG
1	B	510	ARG
1	B	512	THR
1	B	542	LYS
1	B	555	SER

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Mol	Chain	Res	Type
1	B	585	LYS
1	B	592	ASN
1	B	607	LYS
1	B	616	LEU
1	B	625	SER
1	B	628	ILE
1	B	639	ARG
1	B	643	SER
1	B	647	SER
1	B	660	GLU
1	B	667	GLU
1	B	708	LYS
2	E	367	THR
2	E	372	ASN
1	C	7	VAL
1	C	9	LYS
1	C	16	ARG
1	C	24	ARG
1	C	39	SER
1	C	45	SER
1	C	51	ASP
1	C	54	LYS
1	C	56	SER
1	C	59	HIS
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
1	C	92	LYS
1	C	118	HIS
1	C	149	LYS
1	C	189	ARG
1	C	204	LYS
1	C	220	ARG
1	C	224	SER
1	C	225	CYS
1	C	249	SER
1	C	260	ARG
1	C	269	ARG
1	C	276	THR
1	C	290	LYS
1	C	317	LEU
1	C	323	ARG

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Mol	Chain	Res	Type
1	C	325	VAL
1	C	361	VAL
1	C	364	LEU
1	C	384	LYS
1	C	386	ASP
1	C	391	GLN
1	C	394	LYS
1	C	396	VAL
1	C	408	SER
1	C	424	SER
1	C	435	GLN
1	C	452	VAL
1	C	465	SER
1	C	474	ASN
1	C	484	LEU
1	C	505	ARG
1	C	510	ARG
1	C	512	THR
1	C	542	LYS
1	C	555	SER
1	C	585	LYS
1	C	592	ASN
1	C	607	LYS
1	C	616	LEU
1	C	625	SER
1	C	628	ILE
1	C	639	ARG
1	C	643	SER
1	C	647	SER
1	C	660	GLU
1	C	667	GLU
1	C	708	LYS
2	F	367	THR
2	F	372	ASN
2	P	2	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	46	HIS
1	A	275	HIS

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Mol	Chain	Res	Type
1	A	328	ASN
1	A	569	ASN
1	A	592	ASN
1	A	630	ASN
1	A	633	ASN
1	A	733	ASN
2	D	372	ASN
1	B	18	ASN
1	B	46	HIS
1	B	275	HIS
1	B	328	ASN
1	B	569	ASN
1	B	592	ASN
1	B	630	ASN
1	B	633	ASN
1	B	733	ASN
2	E	372	ASN
1	C	18	ASN
1	C	46	HIS
1	C	275	HIS
1	C	328	ASN
1	C	569	ASN
1	C	592	ASN
1	C	630	ASN
1	C	633	ASN
1	C	733	ASN
2	F	372	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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	ATP	A	762	-	24,33,33	1.23	3 (12%)	31,52,52	1.18	3 (9%)
3	ATP	B	762	-	24,33,33	1.23	3 (12%)	31,52,52	1.18	2 (6%)
3	ATP	C	762	-	24,33,33	1.23	3 (12%)	31,52,52	1.18	3 (9%)

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	ATP	A	762	-	-	0/18/38/38	0/3/3/3
3	ATP	B	762	-	-	0/18/38/38	0/3/3/3
3	ATP	C	762	-	-	0/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	762	ATP	C8-N7	-3.02	1.28	1.34
3	B	762	ATP	C8-N7	-3.01	1.28	1.34
3	C	762	ATP	C8-N7	-3.01	1.28	1.34
3	A	762	ATP	C5-N7	-2.20	1.31	1.39
3	C	762	ATP	C5-N7	-2.19	1.32	1.39
3	B	762	ATP	C5-N7	-2.19	1.32	1.39
3	C	762	ATP	C2-N1	2.18	1.38	1.33
3	A	762	ATP	C2-N1	2.18	1.38	1.33
3	B	762	ATP	C2-N1	2.19	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	762	ATP	O3A-PA-O5'	-2.54	96.19	102.94
3	B	762	ATP	O3A-PA-O5'	-2.54	96.19	102.94
3	A	762	ATP	O3A-PA-O5'	-2.54	96.20	102.94
3	C	762	ATP	C1'-N9-C4	2.01	129.97	126.94
3	A	762	ATP	C1'-N9-C4	2.01	129.97	126.94
3	B	762	ATP	C4-C5-N7	3.22	112.44	109.48
3	A	762	ATP	C4-C5-N7	3.24	112.46	109.48
3	C	762	ATP	C4-C5-N7	3.28	112.50	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	762	ATP	1	0
3	B	762	ATP	1	0
3	C	762	ATP	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	733/761 (96%)	0.03	31 (4%) 40 16	27, 42, 81, 114	0
1	B	733/761 (96%)	0.07	37 (5%) 32 13	27, 42, 81, 114	0
1	C	733/761 (96%)	0.10	19 (2%) 59 29	27, 42, 81, 114	0
2	D	13/20 (65%)	0.38	2 (15%) 3 1	65, 87, 101, 101	0
2	E	13/20 (65%)	0.64	2 (15%) 3 1	65, 87, 101, 101	0
2	F	13/20 (65%)	0.18	0 100 100	65, 87, 101, 101	0
2	P	3/20 (15%)	-0.17	0 100 100	49, 49, 55, 63	0
All	All	2241/2363 (94%)	0.07	91 (4%) 41 16	27, 42, 87, 114	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	12.0
1	A	271	GLY	7.5
1	A	11	ASP	6.8
1	B	273	ALA	6.3
1	C	271	GLY	6.2
1	B	272	GLU	6.1
1	C	297	VAL	5.8
1	C	272	GLU	5.3
1	A	273	ALA	5.2
1	A	12	GLY	5.2
1	A	297	VAL	5.1
1	B	295	GLY	5.0
1	A	13	SER	4.9
1	B	296	GLY	4.9
1	A	323	ARG	4.8
1	A	269	ARG	4.7
2	E	372	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	607	LYS	4.4
1	B	6	LEU	4.3
1	C	325	VAL	4.0
1	C	265	GLY	3.9
1	A	272	GLU	3.8
1	B	271	GLY	3.7
1	A	296	GLY	3.6
1	B	270	GLY	3.6
1	A	17	ILE	3.5
1	B	18	ASN	3.4
1	C	296	GLY	3.4
1	C	270	GLY	3.4
1	C	298	ARG	3.4
1	B	274	PHE	3.3
1	C	13	SER	3.3
1	B	294	GLN	3.3
1	B	17	ILE	3.1
1	A	736	ASP	3.1
1	C	14	THR	3.1
1	C	295	GLY	3.0
1	A	73	ASP	2.9
1	B	297	VAL	2.9
1	B	323	ARG	2.9
1	C	294	GLN	2.8
1	B	326	GLU	2.8
1	A	74	ALA	2.7
1	B	386	ASP	2.7
1	A	46	HIS	2.7
1	A	298	ARG	2.6
1	B	608	THR	2.6
1	A	10	ARG	2.6
1	B	178	ALA	2.6
1	B	126	GLU	2.6
1	A	52	GLY	2.6
1	B	11	ASP	2.5
1	B	325	VAL	2.5
1	C	16	ARG	2.5
2	E	363	SER	2.5
1	A	9	LYS	2.5
1	B	268	ILE	2.5
1	B	600	GLU	2.4
1	B	610	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	559	ALA	2.4
1	C	15	GLU	2.4
1	A	38	ILE	2.4
1	A	6	LEU	2.4
1	A	18	ASN	2.4
1	C	57	ASP	2.4
1	B	102	LEU	2.4
1	A	15	GLU	2.3
1	A	162	THR	2.3
2	D	372	ASN	2.3
1	A	23	HIS	2.3
1	B	5	LEU	2.3
1	B	598	ASP	2.3
1	A	663	HIS	2.3
1	C	386	ASP	2.3
1	A	120	LEU	2.2
1	C	392	ARG	2.2
1	A	14	THR	2.2
1	B	9	LYS	2.2
1	B	712	GLN	2.2
1	B	14	THR	2.1
1	B	266	SER	2.1
1	A	5	LEU	2.1
1	B	265	GLY	2.1
1	B	269	ARG	2.1
1	B	385	ASP	2.1
1	C	736	ASP	2.1
1	A	275	HIS	2.0
1	B	737	GLY	2.0
1	B	388	ILE	2.0
2	D	374	GLN	2.0
1	C	266	SER	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

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	ATP	C	762	31/31	0.60	0.46	1.34	65,66,78,78	0
3	ATP	A	762	31/31	0.69	0.49	0.78	65,66,78,78	0
3	ATP	B	762	31/31	0.69	0.45	0.76	65,66,78,78	0

6.5 Other polymers

There are no such residues in this entry.