



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 PM GMT

PDB ID : 4B1Z
Title : Structure of the Phactr1 RPEL domain bound to G-actin
Authors : Mouilleron, S.; Wiezlak, M.; O'Reilly, N.; Treisman, R.; Mcdonald, N.Q.
Deposited on : 2012-07-12
Resolution : 3.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (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

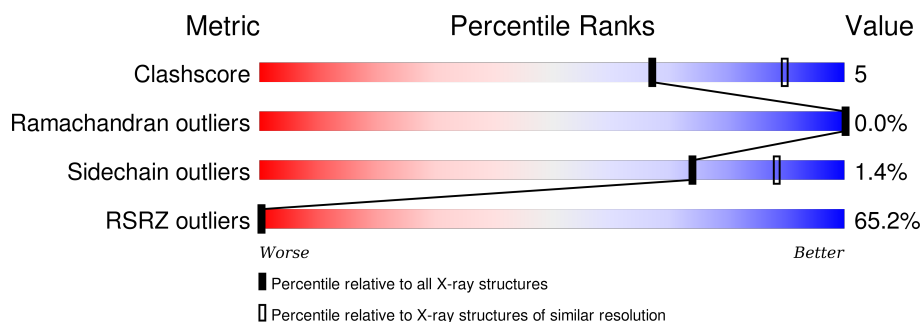
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	<div> <div>63%</div> <div>80%10%11%</div> </div>
1	B	376	<div> <div>67%</div> <div>85%10%5%</div> </div>
1	C	376	<div> <div>61%</div> <div>88%10%.</div> </div>
1	D	376	<div> <div>62%</div> <div>84%11%5%</div> </div>
1	E	376	<div> <div>60%</div> <div>84%12%5%</div> </div>
1	F	376	<div> <div>58%</div> <div>82%13%5%</div> </div>
2	M	115	<div> <div>59%</div> <div>74%18%. .</div> </div>

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Mol	Chain	Length	Quality of chain
2	N	115	

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	1376	-	-	-	X
3	ATP	B	1376	-	-	-	X
3	ATP	C	1376	-	-	-	X
3	ATP	D	1376	-	-	-	X
3	ATP	E	1376	-	-	-	X
3	ATP	F	1376	-	-	-	X
4	MG	D	1377	-	-	-	X
4	MG	E	1377	-	-	-	X
5	GOL	A	1378	-	-	-	X
5	GOL	B	1378	-	-	-	X
5	GOL	C	1378	-	-	-	X
5	GOL	C	1379	-	-	-	X
5	GOL	E	1378	-	-	-	X
5	GOL	N	1529	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17941 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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2495	1588	415	474	18			
1	B	357	Total	C	N	O	S	0	0	0
			2711	1721	448	523	19			
1	C	370	Total	C	N	O	S	0	0	0
			2815	1787	476	532	20			
1	D	356	Total	C	N	O	S	0	0	0
			2648	1675	446	508	19			
1	E	359	Total	C	N	O	S	0	0	0
			2682	1701	450	512	19			
1	F	357	Total	C	N	O	S	0	0	0
			2682	1706	444	513	19			

- Molecule 2 is a protein called PHOSPHATASE AND ACTIN REGULATOR 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	110	Total	C	N	O	0	0	0
			846	517	166	163			
2	N	107	Total	C	N	O	0	0	0
			821	505	159	157			

- 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		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

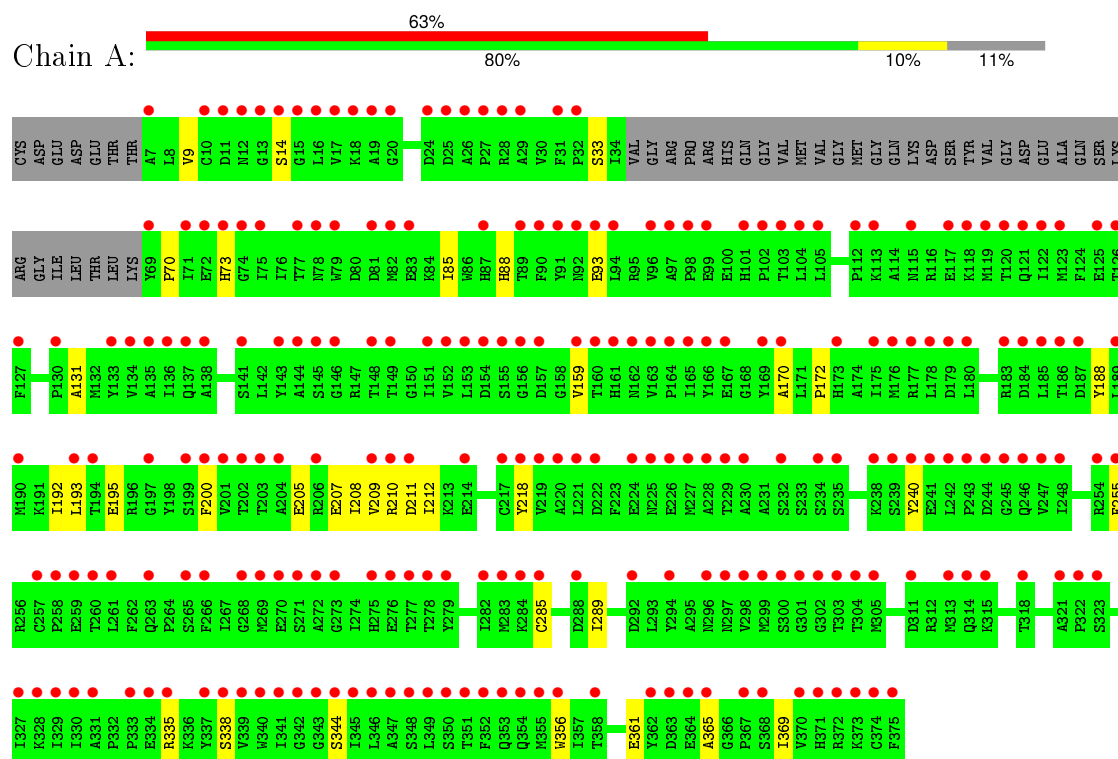
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		

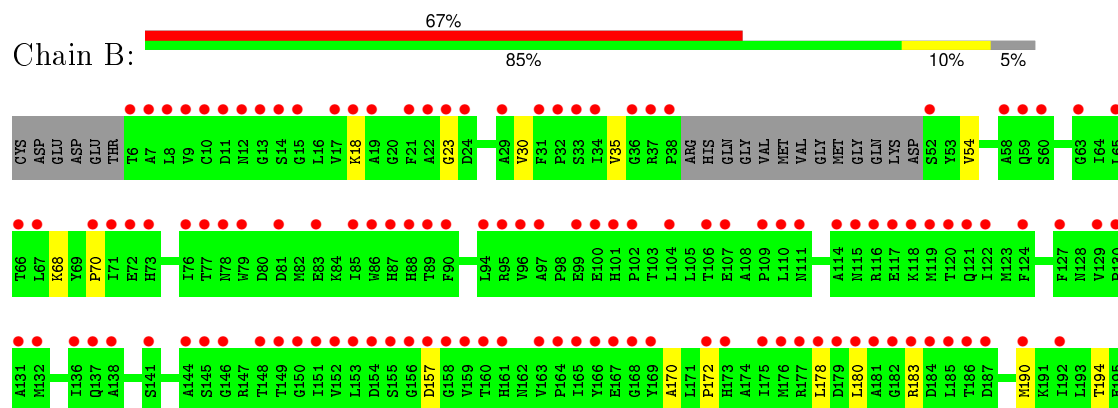
3 Residue-property plots

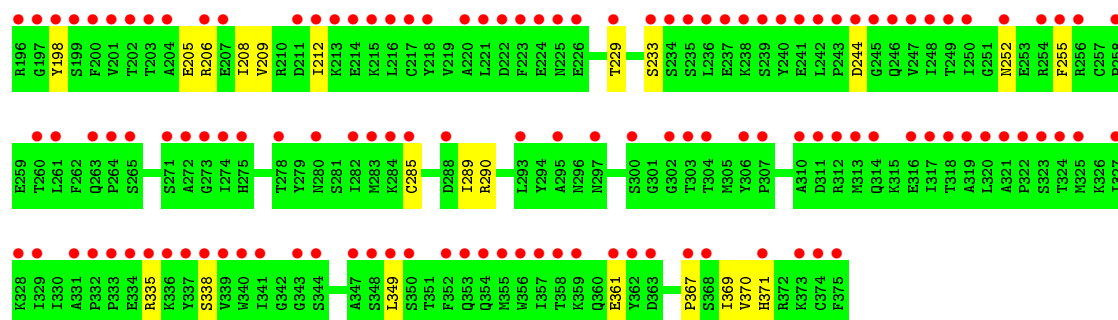
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ACTIN, ALPHA SKELETAL MUSCLE

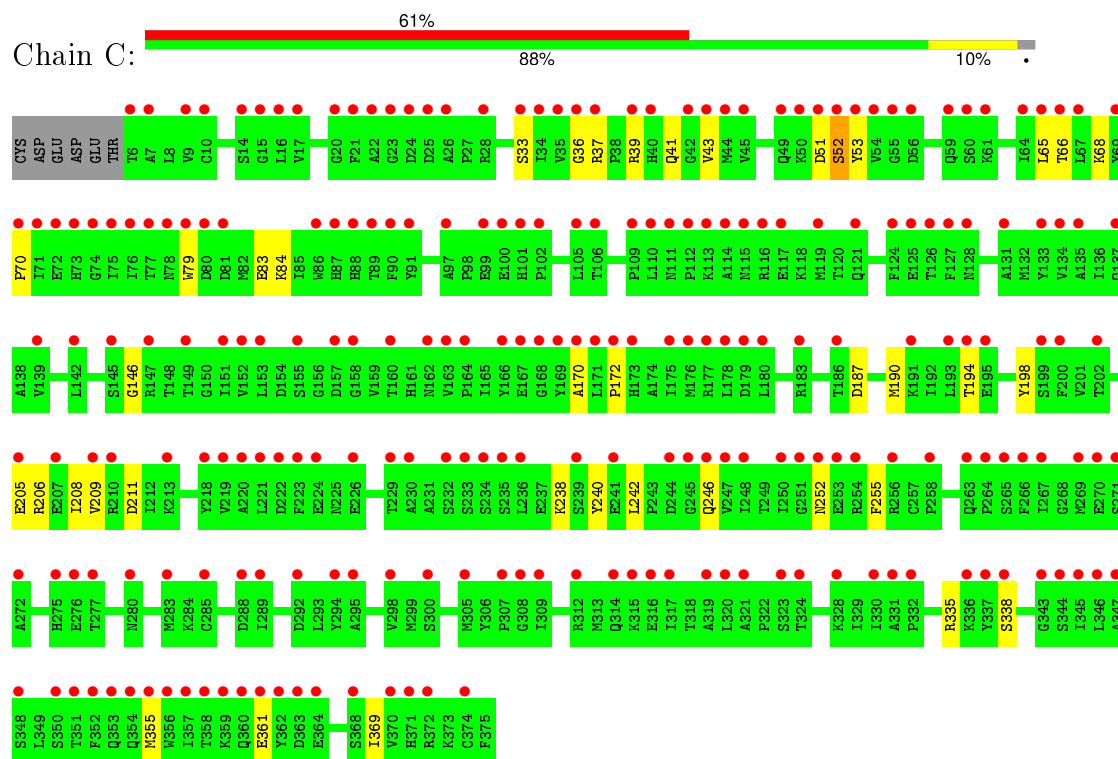


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

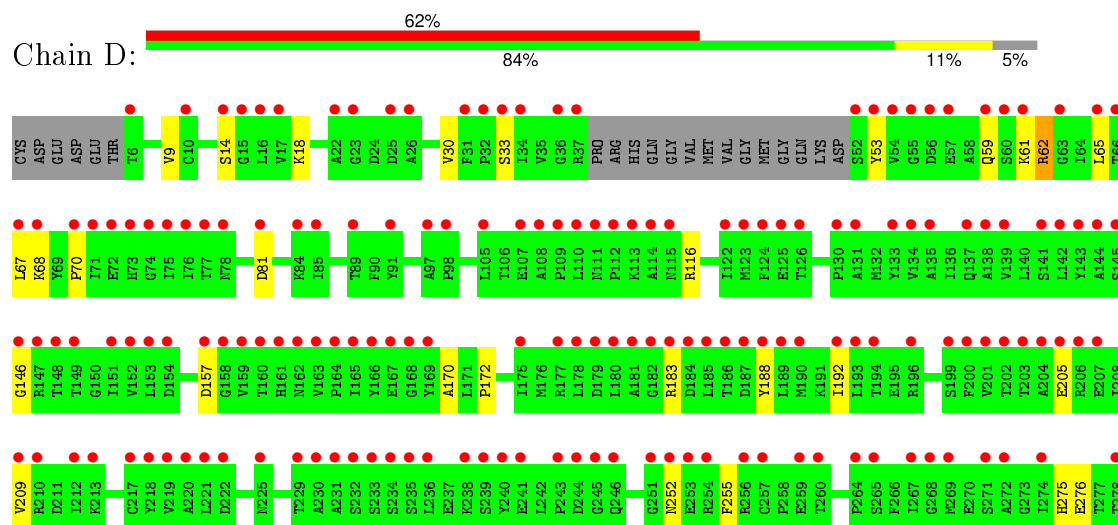


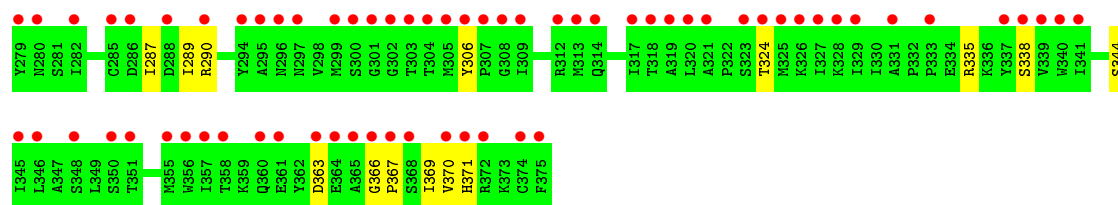


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

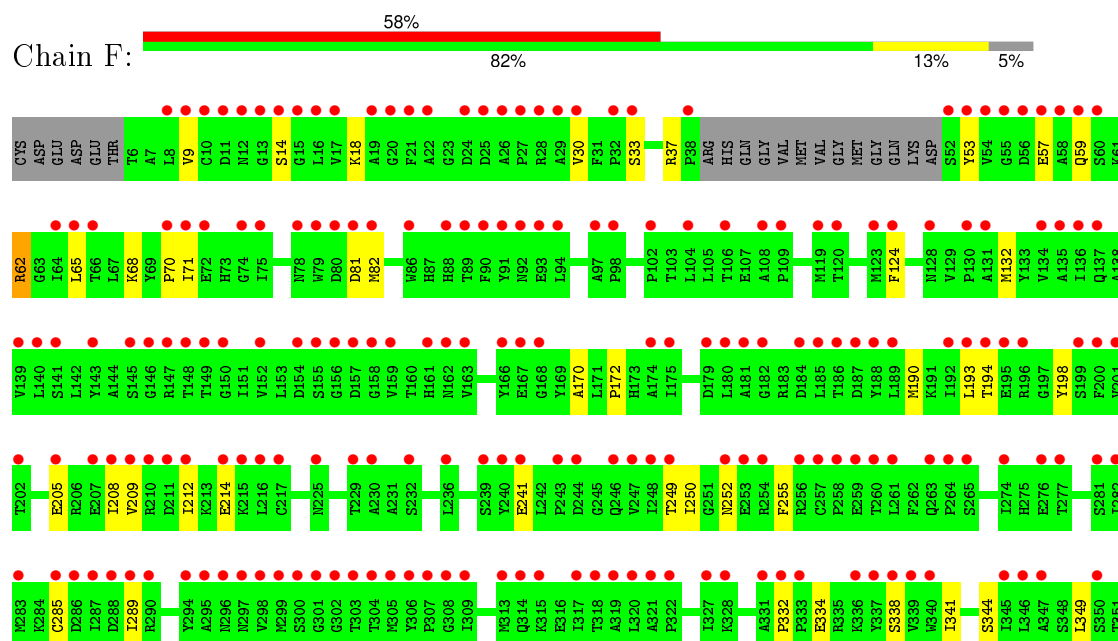


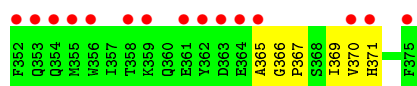


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

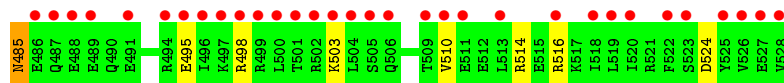
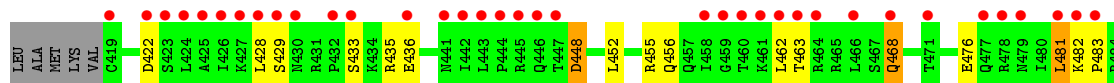
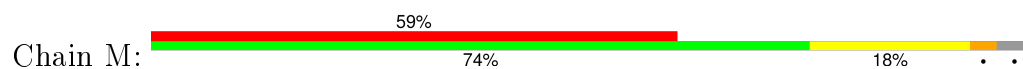


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

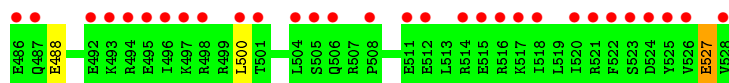
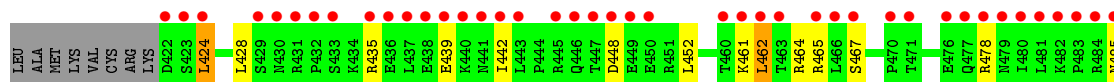
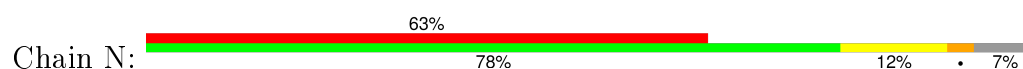




• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.06 Å 142.89 Å 184.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.62 – 3.30 74.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.62-3.30) 99.4 (74.62-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 3.33 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.213 , 0.236 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	6 of 101809 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, 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	0.24	0/2552	0.47	0/3480
1	B	0.24	0/2772	0.46	0/3774
1	C	0.24	0/2878	0.47	0/3911
1	D	0.23	0/2706	0.47	0/3685
1	E	0.24	0/2742	0.47	0/3738
1	F	0.25	0/2742	0.48	0/3736
2	M	0.21	0/851	0.43	0/1148
2	N	0.21	0/827	0.41	0/1115
All	All	0.24	0/18070	0.47	0/24587

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2495	0	2353	19	0
1	B	2711	0	2582	26	0
1	C	2815	0	2724	27	0
1	D	2648	0	2476	26	0
1	E	2682	0	2525	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2682	0	2550	33	0
2	M	846	0	814	13	0
2	N	821	0	787	10	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
3	E	31	0	12	1	0
3	F	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	E	6	0	8	1	0
5	F	6	0	8	0	0
5	N	6	0	8	0	0
6	E	1	0	0	0	0
All	All	17941	0	16947	167	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 5.

All (167) 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:E:146:GLY:O	2:N:465:ARG:NH1	2.04	0.89
1:F:371:HIS:HB3	2:N:527:GLU:HG3	1.58	0.84
1:D:62:ARG:HB2	1:D:67:LEU:HD11	1.63	0.80
1:C:41:GLN:O	1:E:28:ARG:NH2	2.14	0.80
1:C:39:ARG:HG2	1:C:66:THR:HG23	1.67	0.77
1:D:157:ASP:OD2	1:D:183:ARG:NH2	2.27	0.66
1:E:70:PRO:HG3	1:E:81:ASP:HB3	1.77	0.65
1:E:39:ARG:HG2	1:E:66:THR:HG23	1.77	0.65
1:C:246:GLN:HG3	1:F:249:THR:OG1	1.97	0.65
1:B:370:VAL:HG13	1:B:371:HIS:HD2	1.62	0.64
2:M:433:SER:HB3	2:M:436:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:TYR:HD2	1:F:65:LEU:HD21	1.65	0.60
1:D:335:ARG:HA	1:D:338:SER:HB3	1.84	0.60
1:F:53:TYR:CD2	1:F:65:LEU:HD21	2.37	0.59
1:E:370:VAL:HG13	1:E:371:HIS:HD2	1.66	0.59
1:F:190:MET:HG2	1:F:209:VAL:HG21	1.83	0.59
1:D:59:GLN:O	1:D:62:ARG:HB3	2.03	0.58
1:E:199:SER:N	5:E:1378:GOL:O1	2.37	0.58
1:A:335:ARG:HA	1:A:338:SER:HB3	1.85	0.58
1:E:180:LEU:HD21	1:E:260:THR:HG22	1.88	0.56
1:A:14:SER:N	3:A:1376:ATP:O1G	2.26	0.56
1:E:205:GLU:HA	1:E:208:ILE:HG22	1.88	0.55
1:F:59:GLN:O	1:F:62:ARG:HB3	2.07	0.55
1:D:287:ILE:HG12	1:D:290:ARG:NH1	2.23	0.54
1:B:23:GLY:HA2	2:M:455:ARG:NH2	2.22	0.54
1:E:324:THR:HG21	1:F:57:GLU:HA	1.89	0.54
1:B:190:MET:HG2	1:B:209:VAL:HG21	1.89	0.54
1:D:9:VAL:HG21	1:D:344:SER:HA	1.90	0.54
1:F:365:ALA:HB3	1:F:369:ILE:HB	1.89	0.54
2:M:485:ASN:OD1	2:M:485:ASN:N	2.39	0.54
1:E:183:ARG:HG2	1:E:206:ARG:HH22	1.72	0.54
1:F:14:SER:N	3:F:1376:ATP:O1G	2.34	0.54
1:E:207:GLU:HG2	1:E:210:ARG:HH21	1.72	0.54
1:D:146:GLY:HA2	2:N:424:LEU:HD23	1.90	0.54
1:C:53:TYR:HD2	1:C:65:LEU:CD2	2.21	0.53
1:F:70:PRO:HG3	1:F:81:ASP:HB3	1.91	0.53
1:F:241:GLU:OE1	2:N:464:ARG:NH2	2.41	0.53
2:M:510:VAL:HG12	2:M:514:ARG:HE	1.74	0.53
1:F:194:THR:HA	1:F:198:TYR:O	2.09	0.53
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.89	0.53
1:D:324:THR:HG21	1:E:57:GLU:HA	1.91	0.53
1:C:211:ASP:OD2	1:C:240:TYR:OH	2.22	0.52
1:F:332:PRO:HB2	1:F:334:GLU:OE2	2.10	0.52
1:C:36:GLY:O	1:C:52:SER:HA	2.09	0.52
1:D:367:PRO:O	1:D:370:VAL:HG12	2.10	0.52
1:A:365:ALA:HB3	1:A:369:ILE:HB	1.92	0.52
1:D:33:SER:OG	1:D:33:SER:O	2.28	0.52
1:F:170:ALA:O	1:F:172:PRO:HD3	2.11	0.51
1:C:194:THR:HA	1:C:198:TYR:O	2.10	0.51
1:E:306:TYR:CE1	3:E:1376:ATP:H2	2.29	0.51
1:B:349:LEU:HD13	2:M:463:THR:HG23	1.92	0.51
1:F:205:GLU:O	1:F:209:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:O	1:B:70:PRO:HD3	2.11	0.50
1:E:194:THR:HA	1:E:198:TYR:O	2.10	0.50
1:C:205:GLU:O	1:C:209:VAL:HG23	2.12	0.50
1:E:39:ARG:HG3	1:E:65:LEU:HA	1.94	0.50
1:F:33:SER:O	1:F:33:SER:OG	2.28	0.50
1:A:33:SER:OG	1:A:33:SER:O	2.29	0.49
1:E:146:GLY:HA2	2:N:462:LEU:HD23	1.95	0.49
1:C:170:ALA:O	1:C:172:PRO:HD3	2.11	0.49
2:M:495:GLU:OE2	2:M:498:ARG:NH1	2.45	0.49
1:B:194:THR:HA	1:B:198:TYR:O	2.13	0.49
1:E:170:ALA:O	1:E:172:PRO:HD3	2.13	0.49
1:B:18:LYS:HG3	1:B:30:VAL:HG22	1.94	0.48
1:F:18:LYS:HG3	1:F:30:VAL:HG22	1.94	0.48
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.95	0.48
1:E:33:SER:O	1:E:33:SER:OG	2.28	0.48
1:F:214:GLU:O	2:N:478:ARG:NH1	2.39	0.48
1:D:289:ILE:HD11	2:N:442:ILE:HG12	1.94	0.48
1:D:70:PRO:HG3	1:D:81:ASP:HB3	1.95	0.48
1:E:252:ASN:HA	1:E:255:PHE:CE1	2.49	0.48
1:D:14:SER:N	3:D:1376:ATP:O1G	2.32	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.48
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.94	0.47
1:F:349:LEU:HD11	2:N:500:LEU:HD23	1.95	0.47
1:D:188:TYR:O	1:D:192:ILE:HG12	2.14	0.47
1:E:208:ILE:O	1:E:212:ILE:HG13	2.14	0.47
1:E:183:ARG:HG2	1:E:206:ARG:NH2	2.29	0.47
1:F:193:LEU:HD21	1:F:250:ILE:HG13	1.97	0.47
1:C:146:GLY:O	2:M:503:LYS:NZ	2.47	0.47
2:M:452:LEU:O	2:M:456:GLN:HG2	2.14	0.47
1:D:68:LYS:O	1:D:70:PRO:HD3	2.15	0.47
1:B:229:THR:HG23	1:D:367:PRO:HD2	1.96	0.46
1:A:170:ALA:O	1:A:172:PRO:HD3	2.15	0.46
2:N:485:ASN:ND2	2:N:488:GLU:OE1	2.48	0.46
1:E:370:VAL:HG13	1:E:371:HIS:CD2	2.49	0.46
1:E:285:CYS:HB3	1:E:289:ILE:HD11	1.97	0.46
1:E:205:GLU:O	1:E:209:VAL:HG23	2.15	0.46
2:M:482:LYS:HA	2:M:483:PRO:HD3	1.84	0.46
1:F:367:PRO:O	1:F:370:VAL:HG12	2.16	0.46
1:C:36:GLY:HA3	1:C:65:LEU:HD13	1.98	0.46
1:F:252:ASN:HA	1:F:255:PHE:CE1	2.50	0.46
1:A:205:GLU:O	1:A:209:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TYR:HD2	1:D:65:LEU:HD21	1.81	0.46
1:A:208:ILE:O	1:A:212:ILE:HG13	2.16	0.45
1:F:71:ILE:HD11	1:F:82:MET:SD	2.55	0.45
1:D:205:GLU:O	1:D:209:VAL:HG23	2.16	0.45
1:B:361:GLU:HB3	1:B:369:ILE:HD13	1.97	0.45
1:B:370:VAL:HG13	1:B:371:HIS:CD2	2.47	0.45
1:F:68:LYS:O	1:F:70:PRO:HD3	2.17	0.45
1:C:68:LYS:O	1:C:70:PRO:HD3	2.16	0.45
1:B:367:PRO:O	1:B:370:VAL:HG12	2.17	0.45
1:F:208:ILE:O	1:F:212:ILE:HG13	2.16	0.45
1:D:170:ALA:O	1:D:172:PRO:HD3	2.16	0.45
1:F:366:GLY:O	1:F:369:ILE:HG22	2.17	0.45
1:B:178:LEU:HG	1:B:180:LEU:HB3	1.98	0.45
2:M:448:ASP:N	2:M:448:ASP:OD1	2.49	0.45
1:A:73:HIS:HA	1:A:159:VAL:HB	1.97	0.45
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.99	0.45
1:D:252:ASN:HA	1:D:255:PHE:CE1	2.52	0.44
1:B:233:SER:HB2	1:D:363:ASP:HA	1.99	0.44
1:C:361:GLU:HB3	1:C:369:ILE:HD13	1.99	0.44
1:C:33:SER:O	1:C:33:SER:OG	2.29	0.44
1:A:9:VAL:HG21	1:A:344:SER:HA	1.99	0.44
1:C:238:LYS:HD3	2:M:468:GLN:NE2	2.33	0.44
2:M:476:GLU:HG2	2:M:481:LEU:HB3	1.99	0.44
1:D:275:HIS:CE1	1:D:276:GLU:HG3	2.53	0.44
1:F:37:ARG:O	1:F:65:LEU:HB2	2.18	0.44
1:A:211:ASP:OD2	1:A:240:TYR:OH	2.16	0.44
1:C:51:ASP:O	1:C:52:SER:OG	2.26	0.44
1:C:37:ARG:HH22	1:C:84:LYS:HE3	1.83	0.44
1:B:335:ARG:HA	1:B:338:SER:HB3	1.99	0.44
1:C:53:TYR:HD2	1:C:65:LEU:HD21	1.83	0.43
1:C:187:ASP:OD1	1:C:206:ARG:NH2	2.40	0.43
1:E:189:LEU:HD13	1:E:257:CYS:HB2	1.99	0.43
1:E:71:ILE:HD11	1:E:82:MET:SD	2.59	0.43
1:B:35:VAL:HG22	1:B:54:VAL:HG22	2.00	0.43
1:E:324:THR:HG21	1:F:57:GLU:CA	2.48	0.43
1:C:208:ILE:HG21	1:C:242:LEU:HD22	1.99	0.43
1:F:285:CYS:HB3	1:F:289:ILE:HD11	2.02	0.42
1:E:226:GLU:HB3	1:E:255:PHE:CE2	2.54	0.42
1:C:252:ASN:HA	1:C:255:PHE:CE1	2.53	0.42
1:E:335:ARG:HA	1:E:338:SER:HB3	2.01	0.42
1:D:116:ARG:HH12	1:D:371:HIS:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:O	1:B:209:VAL:HG23	2.19	0.42
1:B:285:CYS:HB3	1:B:289:ILE:HD11	2.02	0.42
1:B:349:LEU:HD11	2:M:462:LEU:HD23	2.02	0.42
1:B:252:ASN:HA	1:B:255:PHE:CE1	2.54	0.42
1:F:9:VAL:HG21	1:F:344:SER:HA	2.02	0.42
1:C:335:ARG:HA	1:C:338:SER:HB3	2.01	0.42
1:F:124:PHE:CZ	1:F:132:MET:HG3	2.55	0.42
1:A:88:HIS:CD2	1:A:93:GLU:HG2	2.55	0.42
1:E:68:LYS:O	1:E:70:PRO:HD3	2.20	0.41
1:D:366:GLY:O	1:D:369:ILE:HG22	2.20	0.41
1:E:365:ALA:HB3	1:E:369:ILE:HB	2.02	0.41
1:C:79:TRP:O	1:C:83:GLU:HG3	2.20	0.41
1:B:157:ASP:OD1	3:B:1376:ATP:O3'	2.30	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.02	0.41
1:E:367:PRO:O	1:E:370:VAL:HG12	2.20	0.41
1:B:190:MET:HG3	1:B:209:VAL:HG11	2.01	0.41
2:N:464:ARG:O	2:N:467:SER:OG	2.25	0.41
1:D:306:TYR:CE1	3:D:1376:ATP:H2	2.38	0.41
1:B:285:CYS:O	1:B:290:ARG:NH2	2.42	0.41
1:F:338:SER:HA	1:F:341:ILE:HD12	2.03	0.41
1:C:65:LEU:HD12	1:C:65:LEU:O	2.20	0.41
1:A:207:GLU:CD	1:A:210:ARG:HH21	2.24	0.41
1:F:193:LEU:HA	1:F:193:LEU:HD23	1.95	0.41
1:C:43:VAL:HG22	1:E:28:ARG:HD2	2.01	0.41
1:E:361:GLU:HB3	1:E:369:ILE:HD13	2.03	0.41
1:A:218:TYR:O	1:A:255:PHE:HA	2.21	0.41
1:A:193:LEU:HD13	1:A:200:PHE:CE2	2.56	0.41
1:B:244:ASP:N	1:B:244:ASP:OD1	2.53	0.41
1:B:208:ILE:O	1:B:212:ILE:HG13	2.21	0.41
1:C:53:TYR:CD2	1:C:65:LEU:HD21	2.56	0.41
1:A:361:GLU:HB3	1:A:369:ILE:HD13	2.02	0.41
1:A:188:TYR:O	1:A:192:ILE:HG12	2.20	0.40
1:B:183:ARG:HG2	1:B:206:ARG:NH2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	331/376 (88%)	326 (98%)	5 (2%)	0	100	100
1	B	353/376 (94%)	347 (98%)	6 (2%)	0	100	100
1	C	368/376 (98%)	359 (98%)	8 (2%)	1 (0%)	46	81
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100	100
1	E	355/376 (94%)	348 (98%)	7 (2%)	0	100	100
1	F	353/376 (94%)	346 (98%)	7 (2%)	0	100	100
2	M	108/115 (94%)	105 (97%)	3 (3%)	0	100	100
2	N	105/115 (91%)	102 (97%)	3 (3%)	0	100	100
All	All	2325/2486 (94%)	2279 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/319 (79%)	250 (100%)	1 (0%)	93	96
1	B	281/319 (88%)	281 (100%)	0	100	100
1	C	292/319 (92%)	291 (100%)	1 (0%)	94	98
1	D	264/319 (83%)	262 (99%)	2 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	270/319 (85%)	268 (99%)	2 (1%)	88	94
1	F	274/319 (86%)	273 (100%)	1 (0%)	93	96
2	M	83/111 (75%)	73 (88%)	10 (12%)	6	27
2	N	80/111 (72%)	71 (89%)	9 (11%)	7	30
All	All	1795/2136 (84%)	1769 (99%)	26 (1%)	74	88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	C	355	MET
1	D	61	LYS
1	D	62	ARG
1	E	28	ARG
1	E	297	ASN
1	F	62	ARG
2	M	422	ASP
2	M	428	LEU
2	M	429	SER
2	M	435	ARG
2	M	448	ASP
2	M	468	GLN
2	M	481	LEU
2	M	485	ASN
2	M	516	ARG
2	M	524	ASP
2	N	424	LEU
2	N	428	LEU
2	N	435	ARG
2	N	439	GLU
2	N	448	ASP
2	N	452	LEU
2	N	461	LYS
2	N	462	LEU
2	N	527	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS

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Mol	Chain	Res	Type
1	B	371	HIS
1	E	371	HIS

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 ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	1376	4	24,33,33	0.95	1 (4%)	31,52,52	1.83	5 (16%)
5	GOL	A	1378	-	5,5,5	0.36	0	5,5,5	0.19	0
5	GOL	A	1379	-	5,5,5	0.36	0	5,5,5	0.24	0
3	ATP	B	1376	4	24,33,33	0.94	1 (4%)	31,52,52	1.87	4 (12%)
5	GOL	B	1378	-	5,5,5	0.35	0	5,5,5	0.21	0
3	ATP	C	1376	4	24,33,33	0.95	1 (4%)	31,52,52	1.84	4 (12%)
5	GOL	C	1378	-	5,5,5	0.36	0	5,5,5	0.27	0
5	GOL	C	1379	-	5,5,5	0.35	0	5,5,5	0.26	0
3	ATP	D	1376	4	24,33,33	0.96	1 (4%)	31,52,52	1.79	5 (16%)
3	ATP	E	1376	4	24,33,33	0.97	1 (4%)	31,52,52	1.66	4 (12%)
5	GOL	E	1378	-	5,5,5	0.34	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	F	1376	4	24,33,33	0.94	1 (4%)	31,52,52	1.85	5 (16%)
5	GOL	F	1378	-	5,5,5	0.35	0	5,5,5	0.16	0
5	GOL	N	1529	-	5,5,5	0.35	0	5,5,5	0.25	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	ATP	A	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	A	1378	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1379	-	-	0/4/4/4	0/0/0/0
3	ATP	B	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	B	1378	-	-	0/4/4/4	0/0/0/0
3	ATP	C	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	C	1378	-	-	0/4/4/4	0/0/0/0
5	GOL	C	1379	-	-	0/4/4/4	0/0/0/0
3	ATP	D	1376	4	-	0/18/38/38	0/3/3/3
3	ATP	E	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	E	1378	-	-	0/4/4/4	0/0/0/0
3	ATP	F	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	F	1378	-	-	0/4/4/4	0/0/0/0
5	GOL	N	1529	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1376	ATP	C5-C4	3.04	1.47	1.40
3	F	1376	ATP	C5-C4	3.07	1.47	1.40
3	A	1376	ATP	C5-C4	3.08	1.47	1.40
3	C	1376	ATP	C5-C4	3.10	1.47	1.40
3	D	1376	ATP	C5-C4	3.10	1.47	1.40
3	E	1376	ATP	C5-C4	3.13	1.47	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1376	ATP	N3-C2-N1	-7.01	123.52	128.89
3	B	1376	ATP	N3-C2-N1	-6.94	123.58	128.89
3	C	1376	ATP	N3-C2-N1	-6.88	123.63	128.89
3	A	1376	ATP	N3-C2-N1	-6.74	123.73	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1376	ATP	N3-C2-N1	-6.54	123.89	128.89
3	E	1376	ATP	N3-C2-N1	-5.76	124.48	128.89
3	B	1376	ATP	PA-O3A-PB	-3.84	121.94	132.73
3	C	1376	ATP	PA-O3A-PB	-3.48	122.95	132.73
3	A	1376	ATP	PA-O3A-PB	-3.41	123.15	132.73
3	D	1376	ATP	PA-O3A-PB	-3.38	123.24	132.73
3	B	1376	ATP	C4-C5-N7	-3.34	106.41	109.48
3	E	1376	ATP	C4-C5-N7	-3.27	106.47	109.48
3	E	1376	ATP	PA-O3A-PB	-3.25	123.60	132.73
3	C	1376	ATP	C4-C5-N7	-3.19	106.54	109.48
3	F	1376	ATP	C4-C5-N7	-3.12	106.61	109.48
3	D	1376	ATP	C4-C5-N7	-3.06	106.66	109.48
3	A	1376	ATP	C4-C5-N7	-3.04	106.68	109.48
3	F	1376	ATP	PA-O3A-PB	-3.04	124.20	132.73
3	A	1376	ATP	PB-O3B-PG	-2.70	123.61	132.67
3	B	1376	ATP	PB-O3B-PG	-2.69	123.64	132.67
3	C	1376	ATP	PB-O3B-PG	-2.67	123.71	132.67
3	E	1376	ATP	PB-O3B-PG	-2.61	123.91	132.67
3	D	1376	ATP	PB-O3B-PG	-2.47	124.40	132.67
3	F	1376	ATP	C2'-C1'-N9	-2.44	110.56	114.29
3	F	1376	ATP	PB-O3B-PG	-2.44	124.48	132.67
3	A	1376	ATP	C2'-C1'-N9	-2.35	110.71	114.29
3	D	1376	ATP	C2'-C1'-N9	-2.29	110.79	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1376	ATP	1	0
3	B	1376	ATP	1	0
3	D	1376	ATP	2	0
3	E	1376	ATP	1	0
5	E	1378	GOL	1	0
3	F	1376	ATP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/376 (89%)	3.27	235 (70%) 0 0	57, 83, 142, 192	0
1	B	357/376 (94%)	3.13	251 (70%) 0 0	49, 78, 120, 162	0
1	C	370/376 (98%)	2.93	230 (62%) 0 0	55, 74, 107, 137	0
1	D	356/376 (94%)	2.93	233 (65%) 0 0	70, 98, 133, 162	0
1	E	359/376 (95%)	2.98	226 (62%) 0 0	58, 82, 118, 151	0
1	F	357/376 (94%)	2.88	219 (61%) 0 0	55, 82, 128, 166	0
2	M	110/115 (95%)	3.03	68 (61%) 0 0	61, 84, 128, 150	0
2	N	107/115 (93%)	3.28	72 (67%) 0 0	67, 88, 119, 133	0
All	All	2351/2486 (94%)	3.03	1534 (65%) 0 0	49, 84, 128, 192	0

All (1534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	21.7
1	D	326	LYS	16.0
1	A	97	ALA	14.9
1	E	243	PRO	14.2
1	B	197	GLY	13.7
1	D	230	ALA	12.7
1	F	319	ALA	12.3
1	A	348	SER	12.2
1	A	126	THR	11.9
1	B	241	GLU	11.5
1	F	295	ALA	11.4
1	F	52	SER	11.0
2	N	505	SER	10.9
1	C	51	ASP	10.6
1	C	234	SER	10.6
2	N	422	ASP	10.5

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Mol	Chain	Res	Type	RSRZ
1	C	364	GLU	10.4
1	C	233	SER	10.3
2	M	419	CYS	10.2
1	E	184	ASP	10.1
1	B	182	GLY	10.1
1	C	110	LEU	10.0
1	B	179	ASP	9.9
1	F	364	GLU	9.8
1	A	373	LYS	9.8
1	F	135	ALA	9.7
1	A	157	ASP	9.7
1	D	74	GLY	9.6
1	D	213	LYS	9.6
1	B	198	TYR	9.5
1	A	102	PRO	9.4
1	F	9	VAL	9.4
1	F	19	ALA	9.4
1	B	249	THR	9.4
2	M	422	ASP	9.3
1	D	157	ASP	9.3
1	E	232	SER	9.2
1	C	52	SER	9.2
1	D	239	SER	9.1
1	F	13	GLY	9.1
1	C	292	ASP	9.0
1	A	218	TYR	9.0
1	F	327	ILE	9.0
1	F	346	LEU	9.0
1	F	338	SER	9.0
1	C	371	HIS	8.9
2	N	483	PRO	8.7
1	A	19	ALA	8.7
1	E	252	ASN	8.6
1	A	203	THR	8.6
1	E	164	PRO	8.6
1	A	178	LEU	8.5
1	E	75	ILE	8.4
1	E	183	ARG	8.3
1	E	115	ASN	8.2
1	C	179	ASP	8.2
1	E	36	GLY	8.2
1	A	163	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	TYR	8.2
1	B	244	ASP	8.2
1	E	269	MET	8.1
1	F	10	CYS	8.1
1	B	87	HIS	8.1
1	E	231	ALA	8.0
1	C	235	SER	8.0
1	A	229	THR	7.9
1	B	106	THR	7.9
1	D	53	TYR	7.9
1	C	358	THR	7.9
1	E	63	GLY	7.9
1	E	187	ASP	7.8
1	E	54	VAL	7.8
1	E	235	SER	7.8
1	F	337	TYR	7.8
1	D	207	GLU	7.8
1	F	321	ALA	7.8
1	B	14	SER	7.7
1	A	119	MET	7.7
1	E	234	SER	7.7
1	B	168	GLY	7.6
2	M	526	VAL	7.6
1	F	14	SER	7.6
1	D	303	THR	7.5
1	E	157	ASP	7.5
1	F	21	PHE	7.5
2	M	497	LYS	7.5
2	M	446	GLN	7.5
1	A	26	ALA	7.4
1	E	71	ILE	7.4
1	A	228	ALA	7.4
2	M	501	THR	7.4
2	M	496	ILE	7.4
1	C	236	LEU	7.4
1	F	157	ASP	7.3
2	N	485	ASN	7.3
2	N	481	LEU	7.3
1	B	238	LYS	7.2
1	A	17	VAL	7.2
1	B	323	SER	7.2
1	B	367	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASN	7.2
1	B	88	HIS	7.2
1	C	74	GLY	7.2
1	E	25	ASP	7.1
1	C	87	HIS	7.1
1	B	158	GLY	7.1
2	N	476	GLU	7.1
1	B	12	ASN	7.1
1	E	126	THR	7.1
2	N	470	PRO	7.0
1	D	218	TYR	7.0
1	A	186	THR	7.0
1	A	371	HIS	7.0
2	N	439	GLU	7.0
2	M	428	LEU	7.0
1	B	21	PHE	7.0
1	B	163	VAL	6.9
1	B	242	LEU	6.9
2	N	518	ILE	6.9
1	D	84	LYS	6.9
1	D	161	HIS	6.9
1	F	257	CYS	6.9
1	B	250	ILE	6.8
1	D	25	ASP	6.8
1	E	260	THR	6.8
1	C	45	VAL	6.8
1	E	371	HIS	6.8
1	D	324	THR	6.8
1	F	185	LEU	6.8
2	M	510	VAL	6.8
1	F	149	THR	6.8
1	A	234	SER	6.7
1	F	208	ILE	6.7
1	A	375	PHE	6.7
1	C	285	CYS	6.7
1	D	52	SER	6.7
1	C	44	MET	6.7
1	D	305	MET	6.7
1	D	313	MET	6.7
1	D	229	THR	6.7
1	A	314	GLN	6.7
1	E	244	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
2	N	501	THR	6.6
2	M	426	ILE	6.6
1	C	362	TYR	6.6
1	D	56	ASP	6.6
1	D	285	CYS	6.6
1	E	138	ALA	6.6
1	B	164	PRO	6.6
1	B	77	THR	6.5
1	D	206	ARG	6.5
1	C	100	GLU	6.5
1	C	78	ASN	6.5
1	F	38	PRO	6.5
2	M	527	GLU	6.5
1	B	199	SER	6.5
1	A	351	THR	6.4
1	A	92	ASN	6.4
1	E	355	MET	6.4
1	A	101	HIS	6.4
1	B	100	GLU	6.4
1	C	127	PHE	6.4
1	F	148	THR	6.4
1	F	192	ILE	6.4
1	F	55	GLY	6.4
1	C	128	ASN	6.4
1	D	184	ASP	6.4
1	F	81	ASP	6.4
1	D	307	PRO	6.4
1	B	95	ARG	6.4
1	B	225	ASN	6.4
1	E	367	PRO	6.3
1	C	77	THR	6.3
1	E	368	SER	6.3
1	B	114	ALA	6.3
1	D	323	SER	6.3
1	D	327	ILE	6.3
1	E	95	ARG	6.3
2	N	497	LYS	6.3
1	A	374	CYS	6.3
2	N	508	PRO	6.3
1	F	317	ILE	6.3
2	M	429	SER	6.3
1	A	125	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	82	MET	6.2
1	B	264	PRO	6.2
1	F	276	GLU	6.2
1	C	90	PHE	6.2
1	F	94	LEU	6.2
1	F	59	GLN	6.2
2	N	449	GLU	6.2
1	C	91	TYR	6.2
1	B	273	GLY	6.1
1	F	195	GLU	6.1
1	E	102	PRO	6.1
1	E	111	ASN	6.1
1	A	75	ILE	6.1
1	B	321	ALA	6.1
2	N	525	TYR	6.0
1	C	356	TRP	6.0
1	C	193	LEU	6.0
1	A	164	PRO	6.0
1	F	123	MET	6.0
1	B	178	LEU	6.0
1	B	102	PRO	6.0
1	C	80	ASP	6.0
1	A	243	PRO	6.0
1	E	363	ASP	6.0
1	A	184	ASP	6.0
1	B	154	ASP	6.0
1	A	155	SER	5.9
1	D	219	VAL	5.9
1	E	249	THR	5.9
1	C	288	ASP	5.9
1	F	187	ASP	5.9
1	B	265	SER	5.9
1	D	183	ARG	5.9
1	B	150	GLY	5.9
1	A	367	PRO	5.8
1	D	309	ILE	5.8
1	D	302	GLY	5.8
1	A	11	ASP	5.8
1	C	199	SER	5.8
1	C	246	GLN	5.8
1	D	351	THR	5.8
2	M	500	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	156	GLY	5.8
1	C	106	THR	5.7
1	C	35	VAL	5.7
1	D	163	VAL	5.7
1	F	294	TYR	5.7
2	M	460	THR	5.7
1	A	179	ASP	5.6
1	D	272	ALA	5.6
1	E	10	CYS	5.6
1	C	222	ASP	5.6
1	A	347	ALA	5.6
1	B	236	LEU	5.6
1	E	354	GLN	5.6
1	F	70	PRO	5.6
2	N	423	SER	5.6
1	C	170	ALA	5.6
2	M	463	THR	5.6
1	C	320	LEU	5.6
1	E	7	ALA	5.6
1	A	120	THR	5.6
1	B	157	ASP	5.6
1	B	303	THR	5.5
1	F	106	THR	5.5
1	B	127	PHE	5.5
1	D	314	GLN	5.5
1	C	244	ASP	5.5
1	A	25	ASP	5.5
1	A	372	ARG	5.5
2	N	484	ARG	5.5
1	A	278	THR	5.5
1	E	11	ASP	5.4
2	N	506	GLN	5.4
1	E	356	TRP	5.4
1	C	351	THR	5.4
1	C	223	PHE	5.4
1	E	76	ILE	5.4
1	F	300	SER	5.4
1	C	307	PRO	5.4
1	A	187	ASP	5.4
1	F	90	PHE	5.4
1	A	214	GLU	5.3
1	D	57	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	259	GLU	5.3
1	F	318	THR	5.3
1	A	246	GLN	5.3
1	D	23	GLY	5.3
1	D	202	THR	5.3
1	F	308	GLY	5.3
1	C	337	TYR	5.3
1	D	294	TYR	5.3
1	A	368	SER	5.3
1	C	166	TYR	5.3
1	B	9	VAL	5.3
1	D	31	PHE	5.3
1	D	252	ASN	5.3
1	E	64	ILE	5.3
1	B	67	LEU	5.3
1	E	195	GLU	5.3
1	A	118	LYS	5.3
1	F	309	ILE	5.3
1	A	162	ASN	5.3
2	N	442	ILE	5.3
1	A	335	ARG	5.2
1	B	218	TYR	5.2
1	B	109	PRO	5.2
1	F	196	ARG	5.2
2	N	528	VAL	5.2
1	C	10	CYS	5.2
1	E	283	MET	5.2
2	N	479	ASN	5.2
2	N	500	LEU	5.2
1	F	194	THR	5.2
1	F	12	ASN	5.2
1	C	195	GLU	5.2
1	C	6	THR	5.2
1	C	346	LEU	5.2
1	D	296	ASN	5.2
1	F	30	VAL	5.2
1	D	360	GLN	5.2
1	A	364	GLU	5.1
1	D	364	GLU	5.1
1	A	161	HIS	5.1
1	C	272	ALA	5.1
1	E	310	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
2	M	495	GLU	5.1
1	F	304	THR	5.1
1	B	33	SER	5.1
1	D	185	LEU	5.1
1	E	66	THR	5.1
1	D	297	ASN	5.1
1	F	230	ALA	5.1
1	D	333	PRO	5.1
1	D	55	GLY	5.1
2	M	509	THR	5.1
1	B	66	THR	5.1
1	A	14	SER	5.1
1	F	168	GLY	5.1
1	F	184	ASP	5.1
1	E	224	GLU	5.0
1	A	81	ASP	5.0
1	E	74	GLY	5.0
2	N	504	LEU	5.0
1	A	247	VAL	5.0
1	D	14	SER	5.0
1	E	72	GLU	5.0
1	B	274	ILE	5.0
1	F	365	ALA	5.0
1	F	263	GLN	5.0
1	C	111	ASN	5.0
1	F	186	THR	5.0
2	M	423	SER	5.0
1	A	222	ASP	5.0
1	B	285	CYS	5.0
1	B	60	SER	5.0
1	D	60	SER	5.0
1	A	93	GLU	4.9
1	C	24	ASP	4.9
1	C	232	SER	4.9
1	D	113	LYS	4.9
1	D	212	ILE	4.9
2	M	425	ALA	4.9
1	B	32	PRO	4.9
1	B	186	THR	4.9
1	A	260	THR	4.9
1	E	103	THR	4.9
1	F	212	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	217	CYS	4.9
1	A	322	PRO	4.9
1	B	111	ASN	4.9
1	D	141	SER	4.9
1	F	163	VAL	4.9
1	B	101	HIS	4.9
2	M	525	TYR	4.9
1	F	60	SER	4.9
2	N	495	GLU	4.9
1	C	345	ILE	4.8
2	N	443	LEU	4.8
1	C	56	ASP	4.8
1	B	271	SER	4.8
1	D	240	TYR	4.8
1	E	123	MET	4.8
1	E	291	LYS	4.8
1	F	64	ILE	4.8
1	B	240	TYR	4.8
1	A	263	GLN	4.8
1	B	202	THR	4.8
1	B	70	PRO	4.8
1	D	325	MET	4.8
1	D	220	ALA	4.8
1	E	14	SER	4.8
1	A	225	ASN	4.8
1	D	306	TYR	4.8
1	C	312	ARG	4.7
2	M	445	ARG	4.7
1	E	338	SER	4.7
1	C	15	GLY	4.7
1	C	105	LEU	4.7
1	A	32	PRO	4.7
1	E	297	ASN	4.7
1	F	307	PRO	4.7
1	C	294	TYR	4.7
1	F	97	ALA	4.7
1	C	112	PRO	4.7
1	A	219	VAL	4.7
1	F	297	ASN	4.7
1	B	6	THR	4.7
1	F	136	ILE	4.7
1	F	17	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	194	THR	4.7
1	C	368	SER	4.7
2	N	462	LEU	4.7
1	F	258	PRO	4.7
1	B	110	LEU	4.7
1	B	263	GLN	4.7
1	A	74	GLY	4.7
1	A	345	ILE	4.6
1	B	83	GLU	4.6
1	F	159	VAL	4.6
1	E	180	LEU	4.6
1	B	155	SER	4.6
1	B	207	GLU	4.6
1	D	253	GLU	4.6
1	A	272	ALA	4.6
1	D	246	GLN	4.6
1	E	112	PRO	4.6
1	D	203	THR	4.6
1	A	315	LYS	4.6
1	F	260	THR	4.6
1	D	166	TYR	4.6
1	A	173	HIS	4.6
1	B	10	CYS	4.6
1	C	355	MET	4.6
1	A	146	GLY	4.6
1	E	285	CYS	4.6
1	B	63	GLY	4.5
1	F	155	SER	4.5
1	B	149	THR	4.5
1	C	300	SER	4.5
1	E	245	GLY	4.5
1	A	245	GLY	4.5
1	D	70	PRO	4.5
1	A	226	GLU	4.5
1	A	346	LEU	4.5
1	B	7	ALA	4.5
1	F	24	ASP	4.5
1	C	343	GLY	4.5
1	C	317	ILE	4.5
1	D	147	ARG	4.5
1	E	136	ILE	4.5
1	E	341	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	90	PHE	4.5
2	N	438	GLU	4.5
1	C	248	ILE	4.5
1	C	324	THR	4.5
1	D	22	ALA	4.5
2	N	430	ASN	4.5
1	B	344	SER	4.5
1	E	247	VAL	4.5
1	B	81	ASP	4.5
1	B	363	ASP	4.5
1	D	256	ARG	4.5
1	B	314	GLN	4.5
1	B	145	SER	4.5
1	C	36	GLY	4.5
2	N	496	ILE	4.5
1	E	359	LYS	4.5
1	B	237	GLU	4.5
1	A	12	ASN	4.5
1	D	75	ILE	4.5
1	C	17	VAL	4.4
1	E	8	LEU	4.4
1	C	363	ASP	4.4
1	D	337	TYR	4.4
1	A	248	ILE	4.4
1	B	220	ALA	4.4
1	C	338	SER	4.4
1	A	71	ILE	4.4
1	D	339	VAL	4.4
1	F	305	MET	4.4
1	B	52	SER	4.4
1	D	6	THR	4.4
1	B	258	PRO	4.4
1	A	363	ASP	4.4
1	F	33	SER	4.4
1	E	200	PHE	4.4
2	N	465	ARG	4.4
2	M	522	PHE	4.4
1	A	254	ARG	4.4
1	D	356	TRP	4.4
1	A	255	PHE	4.4
1	C	73	HIS	4.4
1	E	80	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	331	ALA	4.4
1	B	248	ILE	4.4
1	D	329	ILE	4.4
2	N	463	THR	4.3
1	C	26	ALA	4.3
1	E	319	ALA	4.3
1	C	147	ARG	4.3
2	N	446	GLN	4.3
1	A	145	SER	4.3
1	C	277	THR	4.3
1	E	259	GLU	4.3
1	F	356	TRP	4.3
1	C	344	SER	4.3
1	E	70	PRO	4.3
1	D	361	GLU	4.3
1	B	222	ASP	4.3
1	C	171	LEU	4.3
1	F	154	ASP	4.3
1	C	54	VAL	4.3
1	E	246	GLN	4.3
1	C	270	GLU	4.3
1	A	189	LEU	4.3
1	E	120	THR	4.3
1	F	352	PHE	4.3
2	M	462	LEU	4.3
1	F	147	ARG	4.3
1	E	104	LEU	4.3
1	D	374	CYS	4.2
1	E	217	CYS	4.2
2	M	498	ARG	4.2
1	A	265	SER	4.2
1	B	184	ASP	4.2
2	M	477	GLN	4.2
1	A	73	HIS	4.2
1	C	43	VAL	4.2
1	E	340	TRP	4.2
1	E	137	GLN	4.2
1	E	262	PHE	4.2
1	B	358	THR	4.2
1	E	181	ALA	4.2
1	A	154	ASP	4.2
1	D	209	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	M	432	PRO	4.2
1	C	354	GLN	4.2
1	C	89	THR	4.2
1	C	121	GLN	4.2
1	E	357	ILE	4.2
1	B	217	CYS	4.2
1	C	16	LEU	4.2
1	C	352	PHE	4.2
1	A	210	ARG	4.2
1	A	350	SER	4.2
1	F	281	SER	4.2
1	F	15	GLY	4.2
1	C	70	PRO	4.2
1	E	265	SER	4.2
1	B	211	ASP	4.2
1	A	138	ALA	4.1
1	D	85	ILE	4.1
1	E	280	ASN	4.1
1	A	297	ASN	4.1
1	F	20	GLY	4.1
1	D	225	ASN	4.1
2	N	482	LYS	4.1
1	F	82	MET	4.1
1	C	134	VAL	4.1
1	D	288	ASP	4.1
2	N	431	ARG	4.1
1	A	176	MET	4.1
1	B	316	GLU	4.1
1	D	114	ALA	4.1
1	D	144	ALA	4.1
1	E	282	ILE	4.1
1	E	348	SER	4.1
1	F	320	LEU	4.1
1	E	190	MET	4.1
2	M	518	ILE	4.1
1	E	344	SER	4.1
1	E	202	THR	4.1
1	F	28	ARG	4.1
2	N	492	GLU	4.1
1	D	320	LEU	4.1
1	C	25	ASP	4.1
1	B	260	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	310	ALA	4.1
1	B	153	LEU	4.1
2	N	524	ASP	4.1
1	F	289	ILE	4.1
1	E	34	ILE	4.1
2	N	511	GLU	4.1
1	A	194	THR	4.1
1	F	93	GLU	4.0
2	M	487	GLN	4.0
1	D	37	ARG	4.0
1	F	79	TRP	4.0
1	D	130	PRO	4.0
1	D	68	LYS	4.0
1	A	313	MET	4.0
1	D	76	ILE	4.0
1	A	185	LEU	4.0
1	A	149	THR	4.0
1	C	126	THR	4.0
1	C	88	HIS	4.0
1	E	220	ALA	4.0
1	A	276	GLU	4.0
1	D	210	ARG	4.0
1	E	165	ILE	4.0
1	C	241	GLU	4.0
1	D	363	ASP	4.0
1	A	283	MET	4.0
1	A	220	ALA	4.0
1	A	72	GLU	4.0
1	C	113	LYS	4.0
1	A	323	SER	4.0
1	B	176	MET	4.0
1	B	318	THR	4.0
1	F	299	MET	4.0
1	F	328	LYS	3.9
1	D	153	LEU	3.9
1	C	162	ASN	3.9
1	D	222	ASP	3.9
1	B	59	GLN	3.9
1	E	96	VAL	3.9
1	F	354	GLN	3.9
1	E	109	PRO	3.9
1	B	355	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	SER	3.9
1	E	91	TYR	3.9
1	F	128	ASN	3.9
1	B	319	ALA	3.9
1	F	54	VAL	3.9
1	F	285	CYS	3.9
1	C	372	ARG	3.9
1	F	331	ALA	3.9
1	C	71	ILE	3.9
1	D	71	ILE	3.9
1	F	66	THR	3.9
1	A	355	MET	3.9
1	D	328	LYS	3.9
1	C	353	GLN	3.9
1	C	169	TYR	3.8
1	F	130	PRO	3.8
2	M	489	GLU	3.8
1	C	55	GLY	3.8
1	D	15	GLY	3.8
1	A	82	MET	3.8
1	C	357	ILE	3.8
1	F	22	ALA	3.8
2	N	515	GLU	3.8
1	A	292	ASP	3.8
1	F	322	PRO	3.8
1	C	155	SER	3.8
1	A	334	GLU	3.8
1	B	107	GLU	3.8
1	E	364	GLU	3.8
1	A	211	ASP	3.8
1	C	97	ALA	3.8
1	A	160	THR	3.8
1	E	203	THR	3.8
1	E	119	MET	3.8
1	F	232	SER	3.8
2	M	505	SER	3.8
1	C	102	PRO	3.8
1	A	221	LEU	3.8
1	B	201	VAL	3.8
1	D	304	THR	3.8
2	N	471	THR	3.8
1	E	69	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	348	SER	3.8
1	B	368	SER	3.8
2	N	441	ASN	3.8
1	C	145	SER	3.8
1	C	370	VAL	3.8
2	N	467	SER	3.8
1	C	99	GLU	3.8
1	C	323	SER	3.8
1	A	204	ALA	3.8
1	C	200	PHE	3.7
1	A	235	SER	3.7
1	C	164	PRO	3.7
1	D	149	THR	3.7
1	F	65	LEU	3.7
1	E	226	GLU	3.7
1	B	233	SER	3.7
1	C	34	ILE	3.7
1	B	324	THR	3.7
1	E	139	VAL	3.7
1	A	167	GLU	3.7
1	E	182	GLY	3.7
1	D	143	TYR	3.7
1	E	290	ARG	3.7
1	C	22	ALA	3.7
1	A	271	SER	3.7
1	D	33	SER	3.7
1	B	245	GLY	3.7
1	D	205	GLU	3.7
1	C	157	ASP	3.7
1	D	165	ILE	3.7
1	A	127	PHE	3.7
1	A	224	GLU	3.7
1	F	98	PRO	3.7
1	F	180	LEU	3.7
1	C	119	MET	3.7
1	B	215	LYS	3.7
1	B	167	GLU	3.7
1	B	272	ALA	3.7
1	F	274	ILE	3.7
2	M	506	GLN	3.7
1	B	254	ARG	3.7
1	E	58	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	3.6
1	B	322	PRO	3.6
1	C	109	PRO	3.6
1	E	186	THR	3.6
1	A	121	GLN	3.6
1	C	361	GLU	3.6
1	F	80	ASP	3.6
2	N	445	ARG	3.6
1	D	371	HIS	3.6
1	A	298	VAL	3.6
1	D	196	ARG	3.6
2	M	523	SER	3.6
1	A	299	MET	3.6
1	E	81	ASP	3.6
1	C	266	PHE	3.6
1	A	15	GLY	3.6
1	E	230	ALA	3.6
1	A	31	PHE	3.6
1	B	15	GLY	3.6
1	B	311	ASP	3.6
1	D	372	ARG	3.6
1	B	226	GLU	3.6
1	B	17	VAL	3.6
1	E	78	ASN	3.6
1	B	354	GLN	3.6
1	B	23	GLY	3.6
1	E	253	GLU	3.6
1	D	164	PRO	3.6
1	E	127	PHE	3.6
1	E	105	LEU	3.5
1	F	193	LEU	3.5
2	N	466	LEU	3.5
1	E	237	GLU	3.5
2	N	437	LEU	3.5
1	C	245	GLY	3.5
1	F	166	TYR	3.5
1	B	229	THR	3.5
1	D	295	ALA	3.5
1	E	114	ALA	3.5
1	A	232	SER	3.5
1	C	316	GLU	3.5
1	D	282	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	86	TRP	3.5
1	D	160	THR	3.5
1	D	278	THR	3.5
1	A	329	ILE	3.5
1	B	85	ILE	3.5
1	D	268	GLY	3.5
1	D	232	SER	3.5
1	E	329	ILE	3.5
1	A	258	PRO	3.5
1	D	32	PRO	3.5
1	A	240	TYR	3.5
1	D	234	SER	3.5
1	E	311	ASP	3.5
1	E	362	TYR	3.5
1	F	375	PHE	3.5
1	B	79	TRP	3.5
1	C	347	ALA	3.5
1	A	115	ASN	3.5
1	A	148	THR	3.5
1	D	65	LEU	3.5
1	A	18	LYS	3.5
1	E	28	ARG	3.5
2	M	481	LEU	3.5
2	N	526	VAL	3.4
1	B	94	LEU	3.4
1	D	142	LEU	3.4
1	D	221	LEU	3.4
1	B	151	ILE	3.4
1	B	357	ILE	3.4
1	F	161	HIS	3.4
1	B	146	GLY	3.4
1	D	138	ALA	3.4
1	D	346	LEU	3.4
1	C	289	ILE	3.4
2	N	520	ILE	3.4
1	A	89	THR	3.4
1	A	96	VAL	3.4
1	F	162	ASN	3.4
1	C	21	PHE	3.4
1	A	69	TYR	3.4
1	D	182	GLY	3.4
1	F	26	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	181	ALA	3.4
2	M	444	PRO	3.4
1	C	202	THR	3.4
1	C	67	LEU	3.4
2	M	494	ARG	3.4
1	E	134	VAL	3.4
1	F	264	PRO	3.4
1	F	75	ILE	3.4
1	A	344	SER	3.4
1	A	83	GLU	3.4
1	A	99	GLU	3.4
1	B	214	GLU	3.4
1	D	286	ASP	3.4
2	M	436	GLU	3.4
1	D	175	ILE	3.4
1	D	233	SER	3.4
1	E	334	GLU	3.4
1	A	242	LEU	3.4
1	B	341	ILE	3.4
1	E	296	ASN	3.4
1	F	296	ASN	3.4
1	B	65	LEU	3.4
1	E	39	ARG	3.4
1	B	213	LYS	3.4
1	C	9	VAL	3.4
1	F	91	TYR	3.4
1	F	370	VAL	3.4
1	A	266	PHE	3.4
1	D	338	SER	3.4
2	N	433	SER	3.4
1	B	96	VAL	3.4
1	B	307	PRO	3.3
1	E	60	SER	3.3
1	D	151	ILE	3.3
1	A	152	VAL	3.3
1	C	247	VAL	3.3
1	A	79	TRP	3.3
1	E	79	TRP	3.3
1	B	18	LYS	3.3
1	B	148	THR	3.3
1	D	357	ILE	3.3
1	E	61	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	477	GLN	3.3
1	B	185	LEU	3.3
1	E	56	ASP	3.3
1	F	25	ASP	3.3
1	A	78	ASN	3.3
1	E	86	TRP	3.3
1	B	129	VAL	3.3
1	D	108	ALA	3.3
1	E	118	LYS	3.3
1	B	224	GLU	3.3
1	E	313	MET	3.3
1	F	303	THR	3.3
1	E	108	ALA	3.3
1	F	29	ALA	3.3
1	B	192	ILE	3.3
1	C	226	GLU	3.3
1	D	54	VAL	3.3
1	F	139	VAL	3.3
2	M	503	LYS	3.3
1	B	11	ASP	3.3
1	B	302	GLY	3.3
1	C	153	LEU	3.3
1	D	162	ASN	3.3
1	F	53	TYR	3.3
1	F	58	ALA	3.3
1	E	256	ARG	3.3
1	A	365	ALA	3.3
1	E	171	LEU	3.3
1	E	288	ASP	3.3
1	B	297	ASN	3.3
1	A	301	GLY	3.3
1	C	20	GLY	3.3
1	E	327	ILE	3.3
2	M	528	VAL	3.3
1	D	200	PHE	3.3
1	B	221	LEU	3.3
1	B	340	TRP	3.2
1	B	181	ALA	3.2
1	A	159	VAL	3.2
1	E	31	PHE	3.2
1	E	258	PRO	3.2
1	A	269	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	50	LYS	3.2
1	B	337	TYR	3.2
1	D	158	GLY	3.2
1	C	66	THR	3.2
1	A	7	ALA	3.2
1	F	214	GLU	3.2
1	F	124	PHE	3.2
1	C	173	HIS	3.2
1	E	20	GLY	3.2
1	D	112	PRO	3.2
1	E	38	PRO	3.2
1	E	325	MET	3.2
1	A	144	ALA	3.2
1	E	350	SER	3.2
1	C	219	VAL	3.2
1	D	236	LEU	3.2
1	E	365	ALA	3.2
1	B	86	TRP	3.2
1	F	88	HIS	3.2
1	F	158	GLY	3.2
1	A	303	THR	3.2
1	B	300	SER	3.2
1	E	52	SER	3.2
2	M	433	SER	3.2
1	A	201	VAL	3.2
1	C	116	ARG	3.2
1	C	137	GLN	3.2
1	D	290	ARG	3.2
1	F	57	GLU	3.2
1	B	374	CYS	3.2
1	A	209	VAL	3.2
1	A	328	LYS	3.2
1	C	252	ASN	3.1
1	A	358	THR	3.1
1	A	341	ILE	3.1
2	N	498	ARG	3.1
1	C	224	GLU	3.1
1	E	90	PHE	3.1
1	A	273	GLY	3.1
1	B	104	LEU	3.1
1	B	38	PRO	3.1
1	B	141	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	295	ALA	3.1
1	D	279	TYR	3.1
1	E	166	TYR	3.1
1	E	188	TYR	3.1
1	B	34	ILE	3.1
1	B	119	MET	3.1
1	A	338	SER	3.1
2	N	521	ARG	3.1
1	F	189	LEU	3.1
1	A	29	ALA	3.1
1	B	203	THR	3.1
1	F	371	HIS	3.1
1	E	116	ARG	3.1
1	D	154	ASP	3.1
1	D	365	ALA	3.1
1	A	337	TYR	3.1
1	B	338	SER	3.1
1	B	375	PHE	3.1
1	B	212	ILE	3.1
1	D	274	ILE	3.1
1	E	298	VAL	3.1
1	D	181	ALA	3.1
1	B	76	ILE	3.1
1	E	287	ILE	3.1
1	B	280	ASN	3.1
1	F	347	ALA	3.1
1	B	362	TYR	3.1
2	M	430	ASN	3.1
1	D	152	VAL	3.1
1	D	243	PRO	3.1
1	F	358	THR	3.1
1	C	359	LYS	3.1
1	D	111	ASN	3.1
1	B	8	LEU	3.1
1	B	353	GLN	3.1
2	M	468	GLN	3.1
1	E	177	ARG	3.1
1	B	256	ARG	3.1
1	B	343	GLY	3.1
1	C	183	ARG	3.1
1	A	137	GLN	3.1
1	E	248	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	27	PRO	3.1
1	B	235	SER	3.0
1	F	141	SER	3.0
1	C	65	LEU	3.0
1	A	340	TRP	3.0
1	B	334	GLU	3.0
1	B	347	ALA	3.0
1	B	339	VAL	3.0
1	F	333	PRO	3.0
1	C	186	THR	3.0
1	B	349	LEU	3.0
1	C	72	GLU	3.0
2	M	488	GLU	3.0
1	C	321	ALA	3.0
1	E	89	THR	3.0
1	A	156	GLY	3.0
1	E	59	GLN	3.0
2	M	478	ARG	3.0
1	E	330	ILE	3.0
1	D	235	SER	3.0
1	C	79	TRP	3.0
1	D	97	ALA	3.0
1	F	201	VAL	3.0
1	C	210	ARG	3.0
1	E	372	ARG	3.0
1	A	202	THR	3.0
1	C	221	LEU	3.0
1	E	35	VAL	3.0
1	B	31	PHE	3.0
1	F	217	CYS	3.0
2	M	447	THR	3.0
1	D	123	MET	3.0
1	F	298	VAL	3.0
1	D	366	GLY	3.0
1	E	276	GLU	3.0
1	A	143	TYR	3.0
1	E	53	TYR	3.0
1	A	227	MET	3.0
1	B	156	GLY	3.0
1	D	259	GLU	3.0
1	F	350	SER	3.0
1	A	27	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	133	TYR	3.0
1	A	238	LYS	3.0
1	B	247	VAL	3.0
1	E	18	LYS	3.0
1	E	358	THR	3.0
2	N	460	THR	3.0
1	C	23	GLY	3.0
1	D	10	CYS	3.0
1	A	166	TYR	2.9
1	E	346	LEU	2.9
1	D	241	GLU	2.9
1	E	83	GLU	2.9
1	A	239	SER	2.9
1	F	32	PRO	2.9
2	N	523	SER	2.9
1	A	117	GLU	2.9
1	C	328	LYS	2.9
1	E	307	PRO	2.9
1	F	16	LEU	2.9
1	E	286	ASP	2.9
2	N	448	ASP	2.9
1	C	250	ILE	2.9
1	A	277	THR	2.9
1	D	186	THR	2.9
2	N	440	LYS	2.9
1	C	69	TYR	2.9
1	F	240	TYR	2.9
1	F	361	GLU	2.9
1	B	71	ILE	2.9
1	D	63	GLY	2.9
1	F	306	TYR	2.9
1	C	14	SER	2.9
1	B	284	LYS	2.9
1	D	137	GLN	2.9
1	B	283	MET	2.9
1	A	133	TYR	2.9
1	C	115	ASN	2.9
1	C	163	VAL	2.9
1	E	9	VAL	2.9
1	D	135	ALA	2.9
1	E	345	ILE	2.9
1	E	292	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	118	LYS	2.9
1	E	113	LYS	2.9
1	F	315	LYS	2.9
1	A	342	GLY	2.9
1	A	343	GLY	2.9
1	C	39	ARG	2.9
1	D	375	PHE	2.9
1	B	152	VAL	2.9
1	E	241	GLU	2.9
1	B	131	ALA	2.9
1	B	317	ILE	2.9
1	E	366	GLY	2.9
1	F	252	ASN	2.9
1	F	287	ILE	2.9
1	F	332	PRO	2.9
1	A	16	LEU	2.9
1	F	89	THR	2.9
1	F	209	VAL	2.9
1	E	73	HIS	2.9
1	F	78	ASN	2.8
2	M	427	LYS	2.8
1	A	354	GLN	2.8
1	A	356	TRP	2.8
1	A	177	ARG	2.8
1	A	327	ILE	2.8
1	D	267	ILE	2.8
2	M	424	LEU	2.8
1	D	367	PRO	2.8
1	C	229	THR	2.8
1	F	74	GLY	2.8
1	D	331	ALA	2.8
1	B	371	HIS	2.8
1	F	288	ASP	2.8
1	E	32	PRO	2.8
1	C	308	GLY	2.8
1	D	168	GLY	2.8
1	E	6	THR	2.8
1	D	178	LEU	2.8
1	B	328	LYS	2.8
1	C	49	GLN	2.8
1	C	254	ARG	2.8
1	D	179	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	247	VAL	2.8
1	D	189	LEU	2.8
2	N	522	PHE	2.8
1	E	206	ARG	2.8
2	M	520	ILE	2.8
1	B	261	LEU	2.8
1	B	234	SER	2.8
1	A	370	VAL	2.8
2	N	478	ARG	2.8
1	C	125	GLU	2.8
1	B	121	GLN	2.8
1	A	244	ASP	2.8
1	C	37	ARG	2.8
1	E	309	ILE	2.8
1	F	207	GLU	2.8
1	D	321	ALA	2.8
1	A	305	MET	2.8
1	F	119	MET	2.8
1	A	349	LEU	2.8
1	E	316	GLU	2.8
1	A	257	CYS	2.7
1	A	135	ALA	2.7
1	D	139	VAL	2.7
1	B	282	ILE	2.7
1	E	270	GLU	2.7
1	F	167	GLU	2.7
2	M	511	GLU	2.7
1	E	306	TYR	2.7
1	B	350	SER	2.7
1	C	33	SER	2.7
1	C	374	CYS	2.7
1	E	201	VAL	2.7
1	B	13	GLY	2.7
2	M	459	GLY	2.7
1	F	253	GLU	2.7
2	M	464	ARG	2.7
1	C	264	PRO	2.7
1	E	204	ALA	2.7
1	E	233	SER	2.7
1	E	281	SER	2.7
1	F	301	GLY	2.7
1	C	207	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	72	GLU	2.7
1	B	204	ALA	2.7
1	E	302	GLY	2.7
1	B	246	GLN	2.7
1	B	329	ILE	2.7
1	F	140	LEU	2.7
2	N	512	GLU	2.7
1	B	115	ASN	2.7
1	C	280	ASN	2.7
1	F	143	TYR	2.7
1	D	231	ALA	2.7
1	C	139	VAL	2.7
2	N	461	LYS	2.7
1	C	251	GLY	2.7
1	C	253	GLU	2.7
1	E	193	LEU	2.7
1	F	363	ASP	2.7
1	D	98	PRO	2.7
1	B	183	ARG	2.7
1	B	200	PHE	2.7
1	E	132	MET	2.7
1	E	227	MET	2.7
1	D	257	CYS	2.7
1	B	117	GLU	2.7
1	C	315	LYS	2.7
1	F	314	GLN	2.7
1	A	104	LEU	2.7
1	C	158	GLY	2.7
1	D	131	ALA	2.7
1	A	279	TYR	2.6
1	A	318	THR	2.7
1	D	126	THR	2.7
1	D	260	THR	2.7
1	A	141	SER	2.6
1	B	173	HIS	2.6
1	C	271	SER	2.6
1	E	158	GLY	2.6
1	B	206	ARG	2.6
2	M	458	ILE	2.6
1	A	112	PRO	2.6
1	B	137	GLN	2.6
1	C	263	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	153	LEU	2.6
1	B	223	PHE	2.6
1	D	73	HIS	2.6
1	A	190	MET	2.6
1	B	90	PHE	2.6
1	F	8	LEU	2.6
1	B	89	THR	2.6
1	F	345	ILE	2.6
1	B	313	MET	2.6
1	E	209	VAL	2.6
1	A	105	LEU	2.6
1	D	81	ASP	2.6
1	D	177	ARG	2.6
1	B	29	ALA	2.6
1	D	91	TYR	2.6
1	F	244	ASP	2.6
1	D	204	ALA	2.6
1	E	37	ARG	2.6
1	C	205	GLU	2.6
1	D	124	PHE	2.6
1	F	241	GLU	2.6
1	B	169	TYR	2.6
1	A	294	TYR	2.6
1	B	144	ALA	2.6
1	F	174	ALA	2.6
1	C	124	PHE	2.6
1	F	202	THR	2.6
1	D	59	GLN	2.6
1	A	217	CYS	2.6
1	B	73	HIS	2.6
1	F	359	LYS	2.6
1	A	130	PRO	2.6
1	A	206	ARG	2.6
1	C	61	LYS	2.6
1	C	176	MET	2.6
1	C	101	HIS	2.6
1	E	67	LEU	2.6
1	A	268	GLY	2.6
1	C	151	ILE	2.6
1	C	314	GLN	2.6
1	E	62	ARG	2.6
1	C	60	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	188	TYR	2.6
1	E	336	LYS	2.6
1	A	311	ASP	2.6
1	A	352	PHE	2.6
1	D	251	GLY	2.6
1	A	28	ARG	2.5
1	D	317	ILE	2.5
1	A	183	ARG	2.5
1	B	333	PRO	2.5
1	E	271	SER	2.5
1	F	109	PRO	2.5
1	B	361	GLU	2.5
1	E	124	PHE	2.5
1	A	300	SER	2.5
1	C	172	PRO	2.5
1	C	348	SER	2.5
1	D	300	SER	2.5
1	F	313	MET	2.5
2	M	486	GLU	2.5
1	A	77	THR	2.5
1	B	36	GLY	2.5
1	C	350	SER	2.5
1	C	64	ILE	2.5
1	A	134	VAL	2.5
1	A	353	GLN	2.5
1	E	97	ALA	2.5
1	E	65	LEU	2.5
2	M	516	ARG	2.5
1	C	276	GLU	2.5
1	D	125	GLU	2.5
1	A	10	CYS	2.5
1	D	169	TYR	2.5
1	F	216	LEU	2.5
1	B	172	PRO	2.5
1	E	172	PRO	2.5
1	F	175	ILE	2.5
1	F	243	PRO	2.5
1	C	336	LYS	2.5
1	D	318	THR	2.5
1	C	319	ALA	2.5
1	E	154	ASP	2.5
1	E	279	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	355	MET	2.5
1	B	130	PRO	2.5
1	C	75	ILE	2.5
2	M	482	LYS	2.5
1	B	136	ILE	2.5
1	C	309	ILE	2.5
1	D	192	ILE	2.5
1	E	289	ILE	2.5
1	D	370	VAL	2.5
1	F	246	GLN	2.5
1	D	280	ASN	2.5
1	D	355	MET	2.5
1	E	216	LEU	2.5
1	C	360	GLN	2.5
1	E	323	SER	2.5
1	F	215	LYS	2.5
1	A	151	ILE	2.5
1	B	132	MET	2.5
1	E	192	ILE	2.5
1	D	134	VAL	2.5
1	E	347	ALA	2.5
1	D	36	GLY	2.5
1	A	175	ILE	2.5
1	E	339	VAL	2.5
1	C	191	LYS	2.5
1	A	230	ALA	2.4
1	A	331	ALA	2.4
1	C	114	ALA	2.4
1	A	169	TYR	2.4
1	B	175	ILE	2.4
1	F	210	ARG	2.4
1	B	352	PHE	2.4
1	B	58	ALA	2.4
1	D	148	THR	2.4
1	A	261	LEU	2.4
1	D	110	LEU	2.4
1	E	293	LEU	2.4
2	M	504	LEU	2.4
2	M	479	ASN	2.4
1	A	302	GLY	2.4
1	B	335	ARG	2.4
1	D	301	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	345	ILE	2.4
1	A	24	ASP	2.4
2	N	424	LEU	2.4
1	D	254	ARG	2.4
1	F	137	GLN	2.4
2	N	494	ARG	2.4
1	B	332	PRO	2.4
1	B	122	ILE	2.4
1	D	180	LEU	2.4
1	F	104	LEU	2.4
1	F	152	VAL	2.4
1	A	270	GLU	2.4
1	C	218	TYR	2.4
1	A	193	LEU	2.4
1	B	190	MET	2.4
1	B	320	LEU	2.4
1	C	135	ALA	2.4
1	D	146	GLY	2.4
1	F	150	GLY	2.4
1	D	122	ILE	2.4
1	C	178	LEU	2.4
1	C	220	ALA	2.4
1	A	304	THR	2.4
1	D	265	SER	2.4
1	F	145	SER	2.4
1	F	286	ASP	2.4
1	D	107	GLU	2.4
1	B	243	PRO	2.4
1	C	142	LEU	2.4
2	N	435	ARG	2.4
1	E	214	GLU	2.4
1	A	136	ILE	2.4
1	F	282	ILE	2.4
1	D	16	LEU	2.4
1	E	145	SER	2.4
2	M	513	LEU	2.4
1	C	42	GLY	2.4
1	C	53	TYR	2.4
1	D	145	SER	2.4
1	E	277	THR	2.4
1	D	299	MET	2.3
1	A	284	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	516	ARG	2.3
2	N	517	LYS	2.3
1	D	72	GLU	2.3
1	B	138	ALA	2.3
1	F	248	ILE	2.3
1	B	336	LYS	2.3
1	C	81	ASP	2.3
1	F	336	LYS	2.3
1	F	182	GLY	2.3
1	C	330	ILE	2.3
1	A	362	TYR	2.3
1	D	61	LYS	2.3
1	C	305	MET	2.3
1	C	167	GLU	2.3
1	E	178	LEU	2.3
1	E	312	ARG	2.3
2	M	491	GLU	2.3
1	A	282	ILE	2.3
1	D	66	THR	2.3
1	F	131	ALA	2.3
1	D	312	ARG	2.3
1	E	92	ASN	2.3
1	B	22	ALA	2.3
1	B	359	LYS	2.3
1	C	213	LYS	2.3
1	B	196	ARG	2.3
1	D	17	VAL	2.3
1	F	239	SER	2.3
1	A	275	HIS	2.3
1	F	362	TYR	2.3
1	D	238	LYS	2.3
1	A	339	VAL	2.3
1	B	19	ALA	2.3
1	C	131	ALA	2.3
1	C	209	VAL	2.3
1	D	319	ALA	2.3
1	E	321	ALA	2.3
1	C	275	HIS	2.3
1	A	123	MET	2.3
1	B	177	ARG	2.3
1	A	165	ILE	2.3
1	F	71	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	442	ILE	2.3
1	A	288	ASP	2.3
1	A	103	THR	2.3
2	M	499	ARG	2.3
1	B	99	GLU	2.3
1	F	120	THR	2.3
1	F	200	PHE	2.3
1	D	109	PRO	2.3
1	F	102	PRO	2.3
1	C	133	TYR	2.3
1	A	87	HIS	2.3
1	D	358	THR	2.3
2	M	466	LEU	2.3
1	D	34	ILE	2.3
2	M	471	THR	2.3
1	B	373	LYS	2.3
1	E	125	GLU	2.3
1	D	264	PRO	2.3
1	C	168	GLY	2.3
1	B	160	THR	2.3
1	E	149	THR	2.3
1	C	258	PRO	2.2
1	C	40	HIS	2.2
1	D	190	MET	2.2
1	C	28	ARG	2.2
1	F	86	TRP	2.2
1	F	340	TRP	2.2
1	A	113	LYS	2.2
2	N	432	PRO	2.2
1	B	37	ARG	2.2
1	F	254	ARG	2.2
1	F	339	VAL	2.2
1	B	239	SER	2.2
1	B	278	THR	2.2
1	E	337	TYR	2.2
1	F	353	GLN	2.2
2	N	436	GLU	2.2
2	M	443	LEU	2.2
1	C	283	MET	2.2
1	F	56	ASP	2.2
2	N	480	ILE	2.2
1	B	161	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	265	SER	2.2
1	D	194	THR	2.2
1	F	236	LEU	2.2
1	A	296	ASN	2.2
1	C	298	VAL	2.2
1	A	321	ALA	2.2
1	A	94	LEU	2.2
1	E	17	VAL	2.2
1	E	332	PRO	2.2
1	C	230	ALA	2.2
1	B	124	PHE	2.2
1	D	67	LEU	2.2
1	C	267	ILE	2.2
2	M	461	LYS	2.2
1	E	106	THR	2.2
1	D	115	ASN	2.2
2	N	487	GLN	2.2
1	D	244	ASP	2.2
1	F	179	ASP	2.2
1	C	117	GLU	2.2
1	D	133	TYR	2.2
1	D	350	SER	2.2
1	D	368	SER	2.2
2	N	447	THR	2.2
1	B	275	HIS	2.2
1	E	274	ILE	2.2
1	D	348	SER	2.2
1	D	89	THR	2.2
2	M	441	ASN	2.2
1	E	275	HIS	2.2
1	C	177	ARG	2.2
1	C	256	ARG	2.2
1	F	205	GLU	2.2
2	N	450	GLU	2.2
1	C	269	MET	2.2
1	A	200	PHE	2.2
1	D	199	SER	2.2
1	F	265	SER	2.2
1	B	120	THR	2.2
1	D	245	GLY	2.2
1	E	160	THR	2.2
1	B	24	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	159	VAL	2.2
1	C	59	GLN	2.1
1	D	271	SER	2.1
1	D	308	GLY	2.1
1	E	128	ASN	2.1
1	F	225	ASN	2.1
2	N	486	GLU	2.1
1	A	13	GLY	2.1
1	B	312	ARG	2.1
1	D	105	LEU	2.1
2	M	519	LEU	2.1
1	C	160	THR	2.1
1	D	77	THR	2.1
2	M	483	PRO	2.1
1	B	187	ASP	2.1
1	D	26	ALA	2.1
1	D	167	GLU	2.1
1	F	11	ASP	2.1
1	F	92	ASN	2.1
1	B	325	MET	2.1
1	D	193	LEU	2.1
1	F	256	ARG	2.1
1	E	360	GLN	2.1
1	A	122	ILE	2.1
1	A	259	GLU	2.1
1	B	327	ILE	2.1
1	F	229	THR	2.1
1	A	197	GLY	2.1
1	B	97	ALA	2.1
1	C	7	ALA	2.1
1	C	331	ALA	2.1
1	F	146	GLY	2.1
1	B	72	GLU	2.1
1	F	134	VAL	2.1
1	B	116	ARG	2.1
1	B	166	TYR	2.1
1	B	255	PHE	2.1
1	F	199	SER	2.1
1	B	293	LEU	2.1
1	B	288	ASP	2.1
1	C	149	THR	2.1
1	D	78	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	5	THR	2.1
1	F	277	THR	2.1
1	E	26	ALA	2.1
1	F	108	ALA	2.1
1	A	241	GLU	2.1
1	D	340	TRP	2.1
1	A	285	CYS	2.1
1	A	20	GLY	2.1
1	D	187	ASP	2.1
1	E	225	ASN	2.1
1	F	249	THR	2.1
1	F	302	GLY	2.1
1	B	180	LEU	2.1
1	B	306	TYR	2.1
1	C	332	PRO	2.1
1	E	218	TYR	2.1
1	C	76	ILE	2.1
1	B	216	LEU	2.1
1	F	283	MET	2.1
1	B	304	THR	2.1
1	F	211	ASP	2.1
1	E	257	CYS	2.1
1	B	165	ILE	2.1
1	C	175	ILE	2.1
1	B	356	TRP	2.1
1	E	261	LEU	2.1
2	N	514	ARG	2.1
1	A	333	PRO	2.1
2	N	493	LYS	2.1
1	D	201	VAL	2.1
1	C	152	VAL	2.0
1	D	159	VAL	2.0
1	E	16	LEU	2.0
1	F	261	LEU	2.0
1	E	33	SER	2.0
1	A	330	ILE	2.0
1	E	250	ILE	2.0
1	F	290	ARG	2.0
2	M	502	ARG	2.0
2	N	429	SER	2.0
1	D	341	ILE	2.0
1	C	180	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	239	SER	2.0
1	D	269	MET	2.0
1	F	188	TYR	2.0
1	A	170	ALA	2.0
1	B	252	ASN	2.0
1	C	295	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ATP	F	1376	31/31	0.56	0.82	1.02	91,91,91,91	0
3	ATP	E	1376	31/31	0.37	0.74	0.83	112,112,112,112	0
5	GOL	C	1378	6/6	0.20	0.69	0.73	68,68,68,68	0
5	GOL	E	1378	6/6	0.35	0.64	0.57	82,82,82,82	0
4	MG	E	1377	1/1	0.67	0.56	0.25	50,50,50,50	0
5	GOL	B	1378	6/6	0.41	0.81	0.19	89,89,89,89	0
3	ATP	A	1376	31/31	0.45	0.64	0.17	99,99,99,99	0
3	ATP	D	1376	31/31	0.50	0.67	0.13	131,131,131,131	0
3	ATP	B	1376	31/31	0.59	0.62	0.04	81,81,81,81	0
5	GOL	C	1379	6/6	0.64	0.54	-0.04	80,80,80,80	0
4	MG	D	1377	1/1	0.50	0.41	-0.37	56,56,56,56	0
5	GOL	N	1529	6/6	0.43	0.41	-0.61	99,99,99,99	0
3	ATP	C	1376	31/31	0.61	0.40	-0.65	84,84,84,84	0
5	GOL	F	1378	6/6	0.55	0.34	-0.87	64,64,64,64	0
5	GOL	A	1378	6/6	0.77	0.42	-1.01	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	F	1377	1/1	0.07	0.27	-2.04	53,53,53,53	0
4	MG	B	1377	1/1	0.64	0.37	-2.16	39,39,39,39	0
4	MG	A	1377	1/1	0.68	0.28	-	42,42,42,42	0
5	GOL	A	1379	6/6	0.56	0.63	-	89,89,89,89	0
4	MG	C	1377	1/1	0.43	0.99	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.