



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:48 PM BST

PDB ID : 4BEB
Title : MUTANT (K220E) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
Authors : Csefalvay, E.; Lapkouski, M.; Guzanova, A.; Csefalvay, L.; Baikova, T.; Shevelev, I.; Janscak, P.; Smatanova, I.K.; Panjikar, S.; Carey, J.; Weiserova, M.; Ettrich, R.
Deposited on : 2013-03-07
Resolution : 2.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

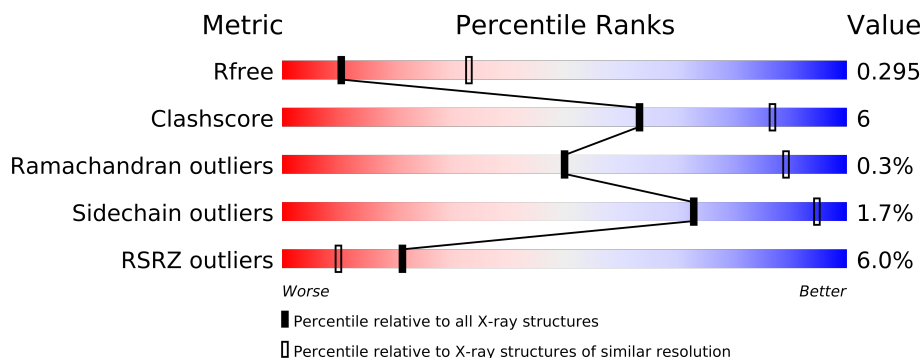
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.99 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}	66092	1468 (3.00-2.96)
Clashscore	79885	1894 (3.00-2.96)
Ramachandran outliers	78287	1826 (3.00-2.96)
Sidechain outliers	78261	1829 (3.00-2.96)
RSRZ outliers	66119	1469 (3.00-2.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1038	
1	B	1038	
1	C	1038	
1	D	1038	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27369 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TYPE I RESTRICTION ENZYME HSDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6821	4340	1158	1307	16			
1	B	842	Total	C	N	O	S	0	0	0
			6846	4353	1158	1319	16			
1	C	838	Total	C	N	O	S	0	0	0
			6802	4326	1151	1309	16			
1	D	833	Total	C	N	O	S	0	0	0
			6772	4309	1146	1301	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
B	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
C	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
D	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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		

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.11Å 123.11Å 160.11Å 90.00° 111.48° 90.00°	Depositor
Resolution (Å)	19.89 – 2.99 19.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.89-2.99) 98.4 (19.88-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.255 , 0.296 0.255 , 0.295	Depositor DCC
R_{free} test set	966 reflections (1.06%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	1.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.6	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	4 of 91281 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27369	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2132e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/6954	0.51	1/9383 (0.0%)
1	B	0.25	0/6979	0.50	1/9418 (0.0%)
1	C	0.27	0/6933	0.49	0/9355
1	D	0.25	0/6901	0.48	1/9309 (0.0%)
All	All	0.26	0/27767	0.50	3/37465 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	VAL	N-CA-C	7.00	129.89	111.00
1	B	813	VAL	N-CA-C	6.66	128.98	111.00
1	D	534	GLY	N-CA-C	5.49	126.81	113.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ALA	Peptide
1	A	769	ILE	Peptide
1	A	806	GLN	Peptide
1	A	812	PRO	Peptide
1	B	144	GLY	Peptide
1	B	769	ILE	Peptide
1	B	806	GLN	Peptide
1	B	812	PRO	Peptide
1	C	769	ILE	Peptide
1	C	806	GLN	Peptide
1	D	769	ILE	Peptide
1	D	811	ASP	Peptide
1	D	812	PRO	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6821	0	6660	83	0
1	B	6846	0	6672	78	0
1	C	6802	0	6636	67	0
1	D	6772	0	6607	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0
All	All	27369	0	26623	297	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (297) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:ALA:HB1	1:A:148:ASN:HA	1.49	0.93
1:A:807:ILE:H	1:A:808:ASP:HB2	1.39	0.86
1:B:807:ILE:H	1:B:808:ASP:HB2	1.44	0.81
1:C:807:ILE:H	1:C:808:ASP:HB2	1.46	0.80
1:D:859:ARG:H	1:D:859:ARG:HH11	1.27	0.79
1:A:365:ALA:HB3	1:C:116:GLU:HB3	1.65	0.79
1:D:819:LYS:NZ	1:D:826:ASP:OD1	2.17	0.78
1:A:810:SER:HB3	1:A:812:PRO:HD3	1.67	0.76
1:B:810:SER:HB3	1:B:812:PRO:HD3	1.65	0.76
1:D:807:ILE:H	1:D:808:ASP:HB2	1.50	0.75
1:A:213:ALA:HB2	1:A:271:VAL:HG23	1.69	0.74
1:B:116:GLU:HB3	1:D:365:ALA:HB3	1.68	0.74
1:C:851:ASN:OD1	1:C:854:ARG:NH1	2.22	0.72
1:D:769:ILE:HG22	1:D:770:GLU:HA	1.70	0.72
1:A:807:ILE:N	1:A:808:ASP:HB2	2.05	0.71
1:C:810:SER:HB3	1:C:812:PRO:HD3	1.74	0.70
1:C:881:ASP:N	1:C:881:ASP:OD1	2.23	0.69
1:A:583:ALA:HB2	1:A:597:GLU:HG2	1.73	0.69
1:A:116:GLU:HB3	1:C:365:ALA:HB3	1.75	0.68
1:C:57:GLN:HE22	1:C:194:LEU:H	1.42	0.68
1:B:807:ILE:N	1:B:808:ASP:HB2	2.09	0.67
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.76	0.67
1:A:94:ASP:OD2	1:A:102:LYS:NZ	2.27	0.66
1:D:154:ILE:HB	1:D:162:VAL:HB	1.75	0.66
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.27	0.66
1:A:811:ASP:H	1:A:814:ALA:HB3	1.60	0.66
1:B:855:ASP:OD1	1:B:858:ARG:NH1	2.28	0.66
1:D:57:GLN:HE22	1:D:194:LEU:H	1.44	0.66
1:B:97:LEU:HD21	1:B:267:GLN:HB3	1.78	0.66
1:C:632:ASN:O	1:C:636:ASN:ND2	2.28	0.66
1:C:812:PRO:HB3	1:C:815:VAL:HB	1.78	0.66
1:A:313:LYS:NZ	1:A:409:GLU:OE2	2.30	0.65
1:B:811:ASP:H	1:B:814:ALA:HB3	1.61	0.65
1:D:532:PHE:O	1:D:534:GLY:HA3	1.97	0.65
1:B:365:ALA:HB3	1:D:116:GLU:HB3	1.78	0.65
1:C:807:ILE:N	1:C:808:ASP:HB2	2.11	0.65
1:B:265:SER:HB3	1:B:352:ARG:HE	1.61	0.64
1:A:632:ASN:O	1:A:636:ASN:ND2	2.30	0.64
1:C:213:ALA:HB2	1:C:271:VAL:HG23	1.79	0.64
1:B:313:LYS:NZ	1:B:409:GLU:OE2	2.30	0.64
1:B:89:LEU:HD11	1:B:159:LEU:HD21	1.79	0.63
1:C:395:ASP:HB3	1:D:836:ARG:HE	1.62	0.63
1:C:125:ASP:OD2	1:C:131:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ASP:OD1	1:A:120:ASN:ND2	2.33	0.62
1:A:154:ILE:HB	1:A:162:VAL:HB	1.82	0.62
1:C:313:LYS:NZ	1:C:409:GLU:OE2	2.26	0.62
1:C:87:GLN:O	1:C:91:ASN:ND2	2.32	0.62
1:D:807:ILE:N	1:D:808:ASP:HB2	2.14	0.61
1:B:819:LYS:NZ	1:B:826:ASP:OD1	2.23	0.61
1:D:40:LEU:HD12	1:D:240:LEU:HD21	1.82	0.61
1:C:613:ASP:OD1	1:C:629:THR:OG1	2.13	0.61
1:B:554:TYR:HB3	1:B:611:PHE:HZ	1.66	0.60
1:B:854:ARG:NH2	1:B:858:ARG:HH22	2.00	0.60
1:A:755:VAL:HG13	1:A:781:LEU:HD22	1.83	0.60
1:B:297:SER:OG	1:B:427:LYS:O	2.14	0.60
1:A:554:TYR:HB3	1:A:611:PHE:HZ	1.67	0.60
1:B:204:SER:HB2	1:B:209:THR:HG23	1.84	0.60
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.83	0.59
1:D:755:VAL:HG13	1:D:781:LEU:HD22	1.84	0.59
1:D:741:THR:HA	1:D:748:ALA:HA	1.82	0.59
1:C:645:VAL:HG21	1:C:653:LEU:HD22	1.83	0.59
1:D:344:TYR:HA	1:D:639:ARG:CZ	2.33	0.59
1:D:541:MET:HG3	1:D:668:LEU:HD11	1.85	0.59
1:D:347:MET:HB2	1:D:639:ARG:NH2	2.17	0.59
1:A:851:ASN:OD1	1:A:854:ARG:NH1	2.35	0.58
1:A:91:ASN:OD1	1:A:91:ASN:N	2.34	0.58
1:C:244:THR:HA	1:C:248:PHE:HB2	1.86	0.57
1:A:763:PHE:HD1	1:A:768:SER:HB3	1.70	0.57
1:D:297:SER:OG	1:D:427:LYS:O	2.16	0.57
1:A:811:ASP:O	1:A:814:ALA:N	2.37	0.57
1:A:581:SER:HB3	1:A:597:GLU:HB3	1.87	0.56
1:D:117:ARG:NH1	1:D:119:GLU:OE2	2.38	0.56
1:B:854:ARG:HH21	1:B:858:ARG:HH22	1.52	0.56
1:B:812:PRO:HA	1:B:814:ALA:H	1.70	0.56
1:C:811:ASP:O	1:C:814:ALA:N	2.34	0.55
1:A:349:GLU:OE2	1:A:352:ARG:NH2	2.30	0.55
1:B:22:LYS:HG3	1:B:242:ASP:OD2	2.06	0.55
1:B:344:TYR:HD1	1:B:639:ARG:HG2	1.70	0.55
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.36	0.55
1:C:776:LYS:HG2	1:C:876:VAL:HG11	1.89	0.55
1:C:154:ILE:HB	1:C:162:VAL:HB	1.89	0.54
1:B:811:ASP:O	1:B:814:ALA:N	2.39	0.54
1:B:645:VAL:HG21	1:B:653:LEU:HD22	1.89	0.54
1:B:244:THR:HA	1:B:248:PHE:HB2	1.89	0.54
1:A:873:TRP:HE3	1:A:876:VAL:HG21	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:554:TYR:HB3	1:C:611:PHE:HZ	1.72	0.53
1:C:54:VAL:HG13	1:C:59:ALA:HB3	1.90	0.53
1:B:745:THR:O	1:B:747:GLU:HB2	2.09	0.53
1:D:769:ILE:CG2	1:D:770:GLU:HA	2.38	0.53
1:B:54:VAL:HG13	1:B:59:ALA:HB3	1.91	0.53
1:C:227:MET:HG2	1:C:273:ARG:HG2	1.89	0.53
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.91	0.53
1:B:162:VAL:HG22	1:B:200:LEU:HB3	1.92	0.52
1:B:462:VAL:HG23	1:B:465:ASP:H	1.73	0.52
1:C:812:PRO:HA	1:C:815:VAL:H	1.75	0.52
1:C:218:ARG:HA	1:C:219:ASP:C	2.30	0.51
1:D:462:VAL:HG23	1:D:465:ASP:H	1.75	0.51
1:D:482:VAL:HG23	1:D:483:ARG:HG3	1.93	0.51
1:C:806:GLN:CB	1:C:807:ILE:HA	2.41	0.51
1:A:490:GLU:HB3	1:A:706:ARG:HA	1.93	0.51
1:D:859:ARG:H	1:D:859:ARG:NH1	2.04	0.50
1:C:91:ASN:N	1:C:91:ASN:OD1	2.36	0.50
1:C:391:LYS:HD3	1:C:417:GLU:OE2	2.11	0.49
1:C:824:VAL:HG13	1:C:828:LYS:HB3	1.94	0.49
1:A:462:VAL:HG23	1:A:465:ASP:H	1.76	0.49
1:A:645:VAL:HG21	1:A:653:LEU:HD22	1.94	0.49
1:A:96:ILE:H	1:A:96:ILE:HD12	1.77	0.49
1:A:695:ALA:HB3	1:A:881:ASP:HB2	1.94	0.49
1:A:812:PRO:HA	1:A:814:ALA:H	1.78	0.49
1:D:804:LEU:HD23	1:D:818:PHE:CE2	2.47	0.49
1:B:154:ILE:HB	1:B:162:VAL:HB	1.94	0.49
1:A:147:ALA:HB1	1:A:148:ASN:CA	2.33	0.49
1:D:204:SER:HB2	1:D:209:THR:HG23	1.95	0.49
1:D:465:ASP:OD1	1:D:468:ARG:NH1	2.44	0.48
1:D:765:ASP:HB2	1:D:766:PRO:HA	1.94	0.48
1:B:772:GLU:HG2	1:B:873:TRP:HE1	1.79	0.48
1:B:695:ALA:HB3	1:B:881:ASP:HB2	1.95	0.48
1:A:303:GLY:O	1:A:432:PHE:HA	2.13	0.48
1:B:355:PRO:HD2	1:B:370:ASN:HD21	1.79	0.48
1:C:384:GLN:HG3	1:C:414:GLN:HG3	1.96	0.48
1:B:71:LEU:O	1:B:131:ARG:NH2	2.41	0.48
1:D:36:LEU:HB3	1:D:166:LEU:HD22	1.95	0.48
1:B:873:TRP:HE3	1:B:876:VAL:HG21	1.78	0.48
1:D:554:TYR:HB3	1:D:611:PHE:HZ	1.79	0.48
1:A:86:GLU:O	1:A:91:ASN:HB3	2.14	0.47
1:D:814:ALA:HA	1:D:817:LYS:HB3	1.94	0.47
1:A:244:THR:HA	1:A:248:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.70	0.47
1:C:162:VAL:HG22	1:C:200:LEU:HB3	1.96	0.47
1:D:384:GLN:HG3	1:D:414:GLN:HG3	1.96	0.47
1:A:125:ASP:OD2	1:A:131:ARG:NH1	2.47	0.47
1:D:770:GLU:O	1:D:775:LYS:NZ	2.48	0.47
1:B:772:GLU:HG3	1:B:856:TRP:HH2	1.78	0.47
1:B:833:GLN:O	1:B:836:ARG:NH2	2.48	0.47
1:B:36:LEU:HB3	1:B:166:LEU:HD22	1.96	0.47
1:C:13:ASN:N	1:C:13:ASN:HD22	2.11	0.47
1:D:313:LYS:NZ	1:D:409:GLU:OE2	2.48	0.47
1:D:806:GLN:CB	1:D:807:ILE:HA	2.45	0.46
1:D:89:LEU:HD11	1:D:159:LEU:HD21	1.97	0.46
1:A:36:LEU:HB3	1:A:166:LEU:HD22	1.97	0.46
1:D:264:ASP:HB2	1:D:349:GLU:OE1	2.15	0.46
1:D:15:ILE:HD11	1:D:277:ILE:HG21	1.96	0.46
1:D:303:GLY:O	1:D:432:PHE:HA	2.15	0.46
1:C:297:SER:OG	1:C:427:LYS:O	2.21	0.46
1:A:63:ASN:O	1:A:67:GLN:HG2	2.15	0.46
1:A:91:ASN:O	1:A:94:ASP:HB2	2.15	0.46
1:A:175:GLU:O	1:A:179:GLN:HG3	2.15	0.46
1:D:509:HIS:CE1	1:D:511:MET:HB2	2.51	0.46
1:C:264:ASP:OD1	1:C:266:SER:OG	2.24	0.46
1:A:807:ILE:HD13	1:A:807:ILE:HA	1.88	0.46
1:B:750:ARG:HH21	1:B:784:GLU:CD	2.19	0.46
1:D:582:PHE:H	1:D:604:MET:HG2	1.80	0.46
1:B:807:ILE:HA	1:B:807:ILE:HD13	1.90	0.46
1:D:298:LYS:HB2	1:D:300:GLU:HG2	1.97	0.46
1:C:792:LEU:HB3	1:C:798:PHE:CG	2.51	0.46
1:B:384:GLN:HG3	1:B:414:GLN:HG3	1.98	0.46
1:C:575:ARG:HD2	1:C:575:ARG:HA	1.71	0.46
1:A:57:GLN:HE21	1:A:57:GLN:HA	1.81	0.46
1:A:824:VAL:HG13	1:A:828:LYS:HB3	1.97	0.46
1:D:402:GLN:NE2	1:D:430:TYR:OH	2.47	0.46
1:B:393:GLU:HB3	1:B:396:LEU:HG	1.98	0.45
1:D:40:LEU:HD12	1:D:166:LEU:HD21	1.96	0.45
1:D:265:SER:HB3	1:D:352:ARG:HE	1.81	0.45
1:A:71:LEU:O	1:A:131:ARG:NH2	2.47	0.45
1:A:769:ILE:HG22	1:A:770:GLU:HA	1.98	0.45
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.97	0.45
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.75	0.45
1:C:691:ARG:HH22	3:C:1886:ATP:PG	2.40	0.45
1:C:128:ASN:ND2	1:C:131:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:36:LEU:HD11	1:D:206:GLY:HA3	1.98	0.45
1:A:344:TYR:HD2	1:A:639:ARG:HG2	1.82	0.45
1:D:63:ASN:O	1:D:67:GLN:HG2	2.17	0.45
1:D:88:TYR:O	1:D:102:LYS:HE2	2.16	0.45
1:C:319:LYS:HD2	1:C:319:LYS:HA	1.76	0.45
1:B:325:THR:HG21	1:B:378:ILE:HB	1.98	0.45
1:B:851:ASN:HA	1:B:854:ARG:NH1	2.32	0.45
1:C:22:LYS:HG3	1:C:242:ASP:OD2	2.16	0.45
1:A:750:ARG:NH1	1:A:758:GLU:OE1	2.50	0.45
1:D:304:TYR:CZ	1:D:457:GLU:HB2	2.52	0.45
1:D:113:PHE:HE1	1:D:119:GLU:HB2	1.83	0.44
1:A:468:ARG:HD2	1:A:469:ASP:OD1	2.17	0.44
1:A:36:LEU:O	1:A:40:LEU:HB2	2.17	0.44
1:C:162:VAL:HG21	1:C:253:LEU:HD11	2.00	0.44
1:B:575:ARG:HD2	1:B:575:ARG:HA	1.71	0.44
1:D:873:TRP:HE3	1:D:876:VAL:HG21	1.82	0.44
1:C:509:HIS:CE1	1:C:511:MET:HB2	2.52	0.44
1:A:296:TRP:NE1	1:A:428:ARG:HG2	2.32	0.44
1:A:471:LYS:HA	1:A:471:LYS:HD3	1.81	0.44
1:D:102:LYS:HA	1:D:106:ASP:HB2	2.00	0.44
1:D:40:LEU:HD11	1:D:164:ILE:HG21	1.99	0.44
1:A:575:ARG:HA	1:A:575:ARG:HD2	1.74	0.44
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.91	0.43
1:D:683:MET:HG3	1:D:719:PHE:CD2	2.53	0.43
1:B:683:MET:HG3	1:B:719:PHE:CD2	2.52	0.43
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.53	0.43
1:B:811:ASP:HA	1:B:812:PRO:HD3	1.76	0.43
1:B:88:TYR:CZ	1:B:109:CYS:HB2	2.53	0.43
1:B:304:TYR:CZ	1:B:457:GLU:HB2	2.53	0.43
1:C:40:LEU:HG	1:C:240:LEU:HD21	2.01	0.43
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.88	0.43
1:B:13:ASN:N	1:B:13:ASN:OD1	2.49	0.43
1:B:229:TRP:CD1	1:B:247:CYS:HB2	2.54	0.43
1:B:427:LYS:HD3	1:B:427:LYS:HA	1.74	0.43
1:C:325:THR:HG21	1:C:378:ILE:HB	1.99	0.43
1:A:833:GLN:O	1:A:836:ARG:NH2	2.52	0.43
1:B:762:ARG:NH2	1:B:777:ASP:HB3	2.34	0.43
1:B:509:HIS:HA	1:B:510:PRO:HD3	1.94	0.43
1:D:18:ASP:HA	1:D:232:SER:OG	2.19	0.43
1:B:264:ASP:HB2	1:B:349:GLU:OE1	2.19	0.43
1:B:91:ASN:HB2	1:B:94:ASP:CG	2.39	0.43
1:C:303:GLY:O	1:C:432:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:391:LYS:HD3	1:D:417:GLU:OE2	2.19	0.43
1:C:395:ASP:HB3	1:D:836:ARG:HB2	2.01	0.43
1:B:873:TRP:O	1:B:876:VAL:HG22	2.19	0.43
1:C:247:CYS:HA	1:C:252:THR:HG21	2.01	0.43
1:D:368:LYS:HB3	1:D:368:LYS:HE2	1.92	0.43
1:B:256:VAL:HA	1:B:260:TYR:HB2	2.00	0.42
1:D:855:ASP:O	1:D:858:ARG:NH1	2.52	0.42
1:A:227:MET:HG2	1:A:273:ARG:HG2	2.01	0.42
1:B:100:THR:HG23	1:B:199:GLN:OE1	2.19	0.42
1:D:873:TRP:O	1:D:876:VAL:HG22	2.20	0.42
1:B:368:LYS:HE2	1:B:368:LYS:HB3	1.77	0.42
1:A:15:ILE:HD11	1:A:277:ILE:HG21	2.01	0.42
1:A:40:LEU:HD12	1:A:166:LEU:HD21	2.01	0.42
1:A:167:LYS:HE3	1:A:176:ALA:HB1	2.01	0.42
1:D:280:THR:HG21	1:D:323:LEU:HD12	2.01	0.42
1:D:745:THR:O	1:D:747:GLU:N	2.52	0.42
1:D:859:ARG:HD3	1:D:859:ARG:H	1.84	0.42
1:A:575:ARG:HE	1:A:622:HIS:CG	2.38	0.42
1:A:684:GLN:O	1:A:688:ARG:NE	2.50	0.42
1:A:687:SER:HB2	1:A:688:ARG:HH21	1.84	0.42
1:A:704:THR:HG21	1:A:708:LEU:HD12	2.01	0.42
1:D:262:VAL:HG21	1:D:315:LEU:HD11	2.01	0.42
1:C:279:ALA:O	1:C:283:ILE:HG13	2.20	0.42
1:A:551:LYS:HA	1:A:611:PHE:CZ	2.55	0.42
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.84	0.42
1:A:99:LYS:HD2	1:A:197:TYR:CE2	2.55	0.42
1:A:850:TYR:CD2	1:A:883:LEU:HD11	2.54	0.42
1:B:337:VAL:O	1:B:382:THR:HA	2.20	0.42
1:B:88:TYR:O	1:B:102:LYS:NZ	2.46	0.42
1:C:36:LEU:HB3	1:C:166:LEU:HD22	2.02	0.42
1:B:303:GLY:O	1:B:432:PHE:HA	2.20	0.42
1:C:765:ASP:HB2	1:C:766:PRO:HA	2.01	0.42
1:C:36:LEU:O	1:C:40:LEU:HB2	2.20	0.41
1:C:755:VAL:HG13	1:C:781:LEU:HD22	2.01	0.41
1:C:551:LYS:HG2	1:C:611:PHE:CG	2.55	0.41
1:C:427:LYS:HD3	1:C:427:LYS:HA	1.76	0.41
1:B:490:GLU:HB3	1:B:706:ARG:HA	2.02	0.41
1:A:467:ILE:HD13	1:A:474:LYS:HG2	2.02	0.41
1:D:792:LEU:HB3	1:D:798:PHE:CG	2.55	0.41
1:A:509:HIS:CE1	1:A:511:MET:HB2	2.55	0.41
1:D:772:GLU:OE2	1:D:873:TRP:NE1	2.42	0.41
1:A:507:PHE:O	1:A:512:ARG:NH1	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:102:LYS:HA	1:B:106:ASP:HB2	2.03	0.41
1:A:30:TYR:HD2	1:A:169:ARG:HD3	1.85	0.41
1:A:54:VAL:HG13	1:A:59:ALA:HB3	2.01	0.41
1:C:482:VAL:O	1:C:484:PRO:HD3	2.20	0.41
1:A:89:LEU:HD11	1:A:159:LEU:HD21	2.01	0.41
1:C:468:ARG:HD2	1:C:469:ASP:OD1	2.20	0.41
1:A:264:ASP:HB2	1:A:349:GLU:OE1	2.20	0.41
1:B:200:LEU:HD13	1:B:271:VAL:HG21	2.03	0.41
1:B:482:VAL:HG23	1:B:483:ARG:HG3	2.01	0.41
1:D:21:ILE:H	1:D:21:ILE:HG12	1.64	0.41
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.86	0.41
1:A:333:VAL:HG22	1:A:404:VAL:HB	2.02	0.41
1:D:171:VAL:O	1:D:205:ASN:ND2	2.40	0.41
1:B:516:ILE:HG23	1:B:705:PHE:CE1	2.56	0.41
1:A:273:ARG:N	1:A:276:GLN:OE1	2.49	0.41
1:A:283:ILE:O	1:A:287:ILE:HG13	2.20	0.41
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.92	0.41
1:A:297:SER:OG	1:A:427:LYS:O	2.26	0.41
1:C:482:VAL:HG23	1:C:483:ARG:HG3	2.03	0.41
1:A:482:VAL:O	1:A:484:PRO:HD3	2.21	0.41
1:A:412:ARG:HG2	1:A:439:ILE:HD11	2.03	0.41
1:A:391:LYS:HD3	1:A:417:GLU:OE2	2.21	0.41
1:C:91:ASN:O	1:C:94:ASP:HB2	2.21	0.41
1:D:334:PHE:HZ	1:D:371:LEU:HD21	1.86	0.41
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.84	0.41
1:C:804:LEU:HD23	1:C:818:PHE:CE2	2.56	0.40
1:D:471:LYS:HD3	1:D:471:LYS:HA	1.83	0.40
1:D:575:ARG:HA	1:D:575:ARG:HD2	1.77	0.40
1:C:520:ILE:O	1:C:524:PHE:HB2	2.21	0.40
1:C:540:ALA:HB2	1:C:670:THR:HB	2.02	0.40
1:A:859:ARG:H	1:A:859:ARG:HG3	1.63	0.40
1:A:769:ILE:CG2	1:A:770:GLU:HA	2.52	0.40
1:B:281:GLU:OE2	1:B:282:ARG:NH1	2.50	0.40
1:A:873:TRP:CE3	1:A:876:VAL:HG21	2.55	0.40
1:C:15:ILE:HB	1:C:252:THR:HG23	2.03	0.40
1:B:262:VAL:HG22	1:B:319:LYS:HD3	2.04	0.40
1:C:304:TYR:CZ	1:C:457:GLU:HB2	2.56	0.40
1:C:368:LYS:HE2	1:C:368:LYS:HB3	1.84	0.40
1:D:581:SER:HB2	1:D:634:PHE:CZ	2.56	0.40
1:B:855:ASP:HA	1:B:858:ARG:HH11	1.86	0.40
1:B:482:VAL:O	1:B:484:PRO:HD3	2.21	0.40
1:B:15:ILE:HD11	1:B:277:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:532:PHE:CG	1:B:533:PRO:HD2	2.57	0.40
1:D:99:LYS:HD2	1:D:197:TYR:CE2	2.56	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	831/1038 (80%)	793 (95%)	36 (4%)	2 (0%)	56	91
1	B	834/1038 (80%)	800 (96%)	32 (4%)	2 (0%)	56	91
1	C	830/1038 (80%)	796 (96%)	33 (4%)	1 (0%)	59	93
1	D	821/1038 (79%)	782 (95%)	35 (4%)	4 (0%)	38	83
All	All	3316/4152 (80%)	3171 (96%)	136 (4%)	9 (0%)	50	89

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	GLY
1	D	813	VAL
1	A	765	ASP
1	C	813	VAL
1	B	813	VAL
1	D	744	ALA
1	A	813	VAL
1	B	765	ASP
1	D	532	PHE

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	737/927 (80%)	724 (98%)	13 (2%)	71	94
1	B	741/927 (80%)	727 (98%)	14 (2%)	69	94
1	C	736/927 (79%)	722 (98%)	14 (2%)	69	94
1	D	733/927 (79%)	725 (99%)	8 (1%)	84	97
All	All	2947/3708 (80%)	2898 (98%)	49 (2%)	73	95

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	40	LEU
1	A	57	GLN
1	A	74	VAL
1	A	91	ASN
1	A	96	ILE
1	A	309	THR
1	A	489	LEU
1	A	507	PHE
1	A	613	ASP
1	A	688	ARG
1	A	781	LEU
1	A	826	ASP
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	57	GLN
1	B	74	VAL
1	B	110	ASP
1	B	215	THR
1	B	326	GLU
1	B	489	LEU
1	B	610	GLU
1	B	613	ASP
1	B	771	SER
1	B	781	LEU
1	B	804	LEU
1	C	13	ASN
1	C	21	ILE
1	C	40	LEU
1	C	74	VAL

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Mol	Chain	Res	Type
1	C	91	ASN
1	C	227	MET
1	C	236	LEU
1	C	507	PHE
1	C	688	ARG
1	C	771	SER
1	C	781	LEU
1	C	827	GLU
1	C	881	ASP
1	C	883	LEU
1	D	21	ILE
1	D	215	THR
1	D	239	ASP
1	D	507	PHE
1	D	753	MET
1	D	781	LEU
1	D	828	LYS
1	D	859	ARG

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

Mol	Chain	Res	Type
1	C	57	GLN
1	D	57	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	A	1886	2	33,33,33	1.04	2 (6%)	52,52,52	1.65	7 (13%)
3	ATP	B	1886	2	33,33,33	1.07	2 (6%)	52,52,52	1.66	9 (17%)
3	ATP	C	1886	2	33,33,33	1.01	2 (6%)	52,52,52	1.72	10 (19%)
3	ATP	D	1886	2	33,33,33	1.04	2 (6%)	52,52,52	1.69	10 (19%)

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	1886	2	-	0/22/38/38	0/1/3/3
3	ATP	B	1886	2	-	0/22/38/38	0/1/3/3
3	ATP	C	1886	2	-	0/22/38/38	0/1/3/3
3	ATP	D	1886	2	-	0/22/38/38	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1886	ATP	C5-C4	3.17	1.47	1.40
3	D	1886	ATP	C5-C4	3.12	1.47	1.40
3	A	1886	ATP	C5-C4	3.04	1.47	1.40
3	C	1886	ATP	C5-C4	3.00	1.47	1.40
3	C	1886	ATP	C4-N9	-2.83	1.33	1.37
3	D	1886	ATP	C4-N9	-2.83	1.33	1.37
3	A	1886	ATP	C4-N9	-2.78	1.33	1.37
3	B	1886	ATP	C4-N9	-2.58	1.34	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1886	ATP	N3-C2-N1	-6.05	123.65	128.71
3	B	1886	ATP	N3-C2-N1	-5.88	123.79	128.71
3	D	1886	ATP	N3-C2-N1	-5.84	123.83	128.71
3	C	1886	ATP	N3-C2-N1	-5.83	123.83	128.71
3	B	1886	ATP	N3-C4-N9	5.33	135.05	125.43
3	C	1886	ATP	N3-C4-N9	5.25	134.91	125.43
3	A	1886	ATP	N3-C4-N9	5.17	134.78	125.43
3	D	1886	ATP	N3-C4-N9	5.09	134.63	125.43
3	B	1886	ATP	C4-C5-N7	-3.52	106.51	109.52
3	D	1886	ATP	C4-C5-N7	-3.49	106.53	109.52
3	C	1886	ATP	C4-C5-N7	-3.37	106.63	109.52
3	A	1886	ATP	C4-C5-N7	-3.28	106.71	109.52
3	D	1886	ATP	PA-O3A-PB	-3.22	122.25	131.68
3	B	1886	ATP	C5-C4-N3	-3.15	118.84	125.70
3	C	1886	ATP	C5-C4-N3	-3.10	118.95	125.70
3	D	1886	ATP	C5-C4-N3	-3.05	119.06	125.70
3	A	1886	ATP	C5-C4-N3	-3.04	119.08	125.70
3	C	1886	ATP	PA-O3A-PB	-2.68	123.81	131.68
3	A	1886	ATP	PA-O3A-PB	-2.62	124.01	131.68
3	C	1886	ATP	C8-N9-C4	2.47	108.79	106.90
3	B	1886	ATP	C8-N9-C4	2.45	108.77	106.90
3	D	1886	ATP	C3'-C2'-C1'	2.43	104.71	100.91
3	A	1886	ATP	C8-N9-C4	2.39	108.73	106.90
3	B	1886	ATP	PA-O3A-PB	-2.35	124.78	131.68
3	D	1886	ATP	C8-N9-C4	2.34	108.69	106.90
3	B	1886	ATP	C2-N3-C4	2.33	120.65	114.01
3	D	1886	ATP	C2-N3-C4	2.29	120.53	114.01
3	A	1886	ATP	C2-N3-C4	2.28	120.50	114.01
3	C	1886	ATP	C2-N3-C4	2.27	120.48	114.01
3	D	1886	ATP	PB-O3B-PG	-2.18	125.28	131.68
3	C	1886	ATP	PB-O3B-PG	-2.18	125.29	131.68
3	C	1886	ATP	O4'-C1'-N9	2.17	110.46	108.44
3	C	1886	ATP	C3'-C2'-C1'	2.17	104.31	100.91
3	B	1886	ATP	O4'-C1'-N9	2.15	110.44	108.44
3	D	1886	ATP	O4'-C1'-N9	2.08	110.37	108.44
3	B	1886	ATP	C3'-C2'-C1'	2.05	104.11	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	839/1038 (80%)	0.01	43 (5%)	27 12	20, 42, 79, 109	0
1	B	842/1038 (81%)	0.28	63 (7%)	14 7	38, 58, 86, 115	0
1	C	838/1038 (80%)	0.01	41 (4%)	28 13	21, 42, 79, 105	0
1	D	833/1038 (80%)	0.37	55 (6%)	18 9	41, 62, 91, 117	0
All	All	3352/4152 (80%)	0.17	202 (6%)	21 10	20, 54, 85, 117	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	767	THR	10.8
1	A	767	THR	8.6
1	C	145	SER	7.2
1	D	583	ALA	6.6
1	C	767	THR	6.4
1	D	767	THR	6.2
1	D	26	THR	5.9
1	D	745	THR	5.7
1	B	810	SER	5.6
1	D	810	SER	5.6
1	D	535	SER	5.5
1	B	744	ALA	5.1
1	D	532	PHE	5.0
1	B	147	ALA	4.9
1	B	146	HIS	4.9
1	D	533	PRO	4.7
1	A	146	HIS	4.7
1	B	144	GLY	4.6
1	A	534	GLY	4.6
1	B	145	SER	4.6
1	C	375	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	859	ARG	4.4
1	A	218	ARG	4.2
1	A	570	THR	4.2
1	C	810	SER	4.2
1	B	148	ASN	4.2
1	B	770	GLU	4.2
1	C	768	SER	4.1
1	D	375	ASP	4.1
1	C	745	THR	4.1
1	B	219	ASP	3.9
1	B	746	GLY	3.9
1	B	446	GLY	3.9
1	C	532	PHE	3.9
1	D	536	LYS	3.9
1	A	810	SER	3.8
1	B	768	SER	3.8
1	A	768	SER	3.7
1	B	26	THR	3.7
1	D	531	THR	3.7
1	C	807	ILE	3.7
1	A	809	LEU	3.7
1	A	624	LYS	3.6
1	A	745	THR	3.6
1	B	217	LYS	3.6
1	A	533	PRO	3.6
1	C	146	HIS	3.5
1	B	747	GLU	3.5
1	A	569	ALA	3.5
1	B	807	ILE	3.5
1	B	215	THR	3.5
1	C	219	ASP	3.5
1	D	219	ASP	3.5
1	D	292	THR	3.4
1	D	140	PHE	3.4
1	D	822	HIS	3.4
1	D	768	SER	3.4
1	A	145	SER	3.4
1	A	816	GLU	3.4
1	C	746	GLY	3.4
1	B	218	ARG	3.3
1	A	766	PRO	3.3
1	B	748	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	743	ALA	3.3
1	C	569	ALA	3.3
1	D	216	THR	3.2
1	D	493	THR	3.2
1	D	570	THR	3.2
1	D	624	LYS	3.2
1	D	179	GLN	3.1
1	B	447	SER	3.1
1	C	217	LYS	3.1
1	B	628	SER	3.1
1	B	808	ASP	3.0
1	B	511	MET	3.0
1	D	571	TYR	3.0
1	D	351	GLN	3.0
1	D	770	GLU	3.0
1	B	356	ASP	2.9
1	A	219	ASP	2.9
1	B	143	ALA	2.9
1	B	841	ARG	2.9
1	B	858	ARG	2.9
1	C	841	ARG	2.9
1	D	807	ILE	2.9
1	A	841	ARG	2.8
1	D	632	ASN	2.8
1	B	534	GLY	2.8
1	A	499	SER	2.8
1	D	840	ASP	2.8
1	B	500	ALA	2.8
1	B	420	LYS	2.8
1	B	533	PRO	2.8
1	C	143	ALA	2.8
1	A	411	HIS	2.7
1	D	29	SER	2.7
1	A	807	ILE	2.7
1	A	345	GLN	2.7
1	B	722	LYS	2.7
1	C	446	GLY	2.7
1	A	144	GLY	2.7
1	D	482	VAL	2.7
1	A	743	ALA	2.7
1	B	772	GLU	2.7
1	B	594	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	841	ARG	2.6
1	A	844	GLN	2.6
1	C	812	PRO	2.6
1	D	617	ARG	2.6
1	A	344	TYR	2.6
1	D	723	ASN	2.6
1	D	722	LYS	2.6
1	A	143	ALA	2.6
1	C	583	ALA	2.6
1	C	770	GLU	2.6
1	A	374	ASP	2.6
1	C	533	PRO	2.6
1	C	218	ARG	2.5
1	D	218	ARG	2.5
1	D	340	LYS	2.5
1	C	855	ASP	2.5
1	B	809	LEU	2.5
1	D	809	LEU	2.5
1	B	569	ALA	2.5
1	B	423	LYS	2.5
1	D	856	TRP	2.5
1	A	772	GLU	2.5
1	C	567	LYS	2.5
1	D	265	SER	2.5
1	B	374	ASP	2.5
1	D	534	GLY	2.5
1	D	747	GLU	2.5
1	C	808	ASP	2.4
1	D	28	ASP	2.4
1	C	772	GLU	2.4
1	B	236	LEU	2.4
1	C	142	GLN	2.4
1	A	769	ILE	2.4
1	C	342	LEU	2.4
1	A	631	SER	2.4
1	B	375	ASP	2.4
1	C	372	ASP	2.4
1	B	445	LEU	2.4
1	C	220	GLU	2.4
1	C	352	ARG	2.3
1	B	593	GLU	2.3
1	D	562	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	115	ASP	2.3
1	B	611	PHE	2.3
1	B	806	GLN	2.3
1	A	147	ALA	2.3
1	C	766	PRO	2.3
1	B	87	GLN	2.3
1	B	456	ARG	2.3
1	C	769	ILE	2.2
1	B	92	PRO	2.2
1	B	344	TYR	2.2
1	D	740	PHE	2.2
1	C	411	HIS	2.2
1	D	766	PRO	2.2
1	A	815	VAL	2.2
1	B	293	ALA	2.2
1	A	808	ASP	2.2
1	A	617	ARG	2.2
1	B	170	GLY	2.2
1	C	593	GLU	2.2
1	D	442	GLU	2.2
1	D	217	LYS	2.2
1	D	579	ILE	2.2
1	B	583	ALA	2.2
1	A	265	SER	2.2
1	D	357	SER	2.2
1	D	413	SER	2.2
1	C	299	PRO	2.2
1	A	744	ALA	2.2
1	C	499	SER	2.1
1	D	769	ILE	2.1
1	B	745	THR	2.1
1	A	375	ASP	2.1
1	A	446	GLY	2.1
1	B	443	ASN	2.1
1	B	567	LYS	2.1
1	C	747	GLU	2.1
1	B	761	GLN	2.1
1	C	806	GLN	2.1
1	C	170	GLY	2.1
1	B	816	GLU	2.1
1	B	827	GLU	2.1
1	B	86	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	855	ASP	2.1
1	D	427	LYS	2.1
1	A	18	ASP	2.0
1	A	765	ASP	2.0
1	D	569	ALA	2.0
1	D	150	TYR	2.0
1	D	537	GLY	2.0
1	B	848	SER	2.0
1	C	744	ALA	2.0
1	B	769	ILE	2.0
1	D	847	ARG	2.0
1	B	859	ARG	2.0
1	C	809	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	1885	1/1	0.21	1.17	52,52,52,52	0
2	MG	A	1885	1/1	0.19	1.03	45,45,45,45	0
2	MG	D	1885	1/1	0.27	0.85	67,67,67,67	0
2	MG	C	1885	1/1	0.15	-0.26	37,37,37,37	0
3	ATP	C	1886	31/31	0.12	-1.22	21,29,39,40	0
3	ATP	D	1886	31/31	0.13	-1.23	45,51,60,62	0
3	ATP	A	1886	31/31	0.12	-1.32	27,34,43,51	0
3	ATP	B	1886	31/31	0.12	-1.39	42,50,57,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.