



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:31 PM GMT

PDB ID : 1HWL
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH ROSUVASTATIN (FORMALLY KNOWN AS ZD4522)
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.10 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>

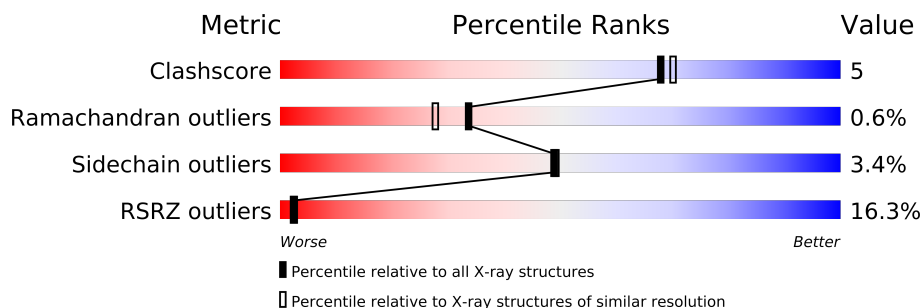
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	467	
1	B	467	
1	C	467	
1	D	467	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12159 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 HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3028	1886	531	581	30			
1	B	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	C	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	D	382	Total	C	N	O	S	0	0	0
			2832	1762	497	544	29			

There are 20 discrepancies between the modelled and reference sequences:

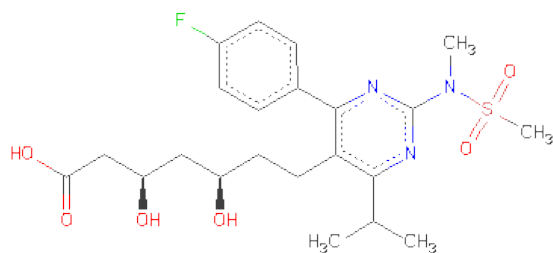
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	INSERTION	UNP P04035
A	423	ALA	-	INSERTION	UNP P04035
A	424	MET	-	INSERTION	UNP P04035
A	425	ALA	-	INSERTION	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	422	GLY	-	INSERTION	UNP P04035
B	423	ALA	-	INSERTION	UNP P04035
B	424	MET	-	INSERTION	UNP P04035
B	425	ALA	-	INSERTION	UNP P04035
B	485	ILE	MET	ENGINEERED	UNP P04035
C	422	GLY	-	INSERTION	UNP P04035
C	423	ALA	-	INSERTION	UNP P04035
C	424	MET	-	INSERTION	UNP P04035
C	425	ALA	-	INSERTION	UNP P04035
C	485	ILE	MET	ENGINEERED	UNP P04035
D	422	GLY	-	INSERTION	UNP P04035
D	423	ALA	-	INSERTION	UNP P04035
D	424	MET	-	INSERTION	UNP P04035
D	425	ALA	-	INSERTION	UNP P04035
D	485	ILE	MET	ENGINEERED	UNP P04035

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is 7-[4-(4-FLUORO-PHENYL)-6-ISOPROPYL-2-(METHANESULFONYL-METHYL-AMINO)-PYRIMIDIN-5-YL]-3,5-DIHYDROXY-HEPTANOICACID (three-letter code: FBI) (formula: $C_{22}H_{30}FN_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	A	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	D	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	C	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		

- Molecule 4 is water.

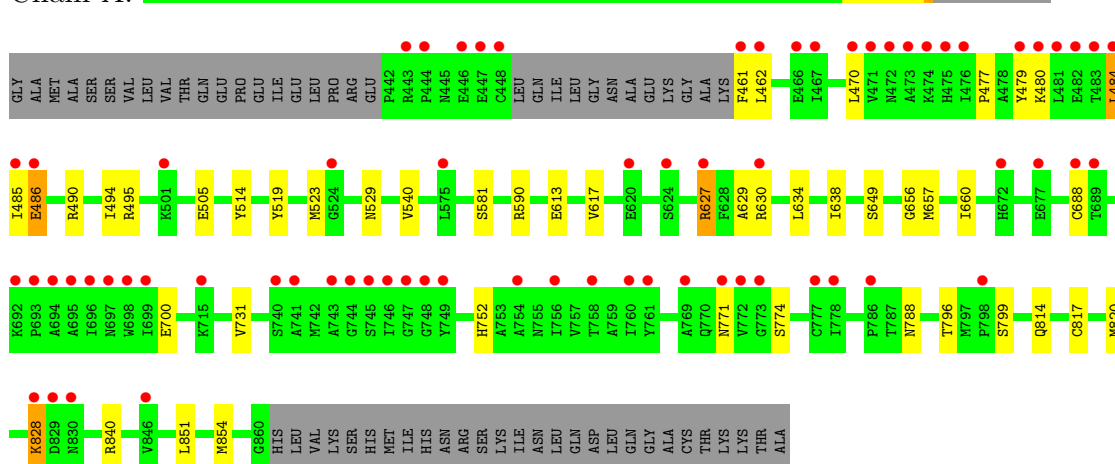
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	41	Total	O	0	0
			41	41		
4	C	44	Total	O	0	0
			44	44		
4	D	48	Total	O	0	0
			48	48		

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.

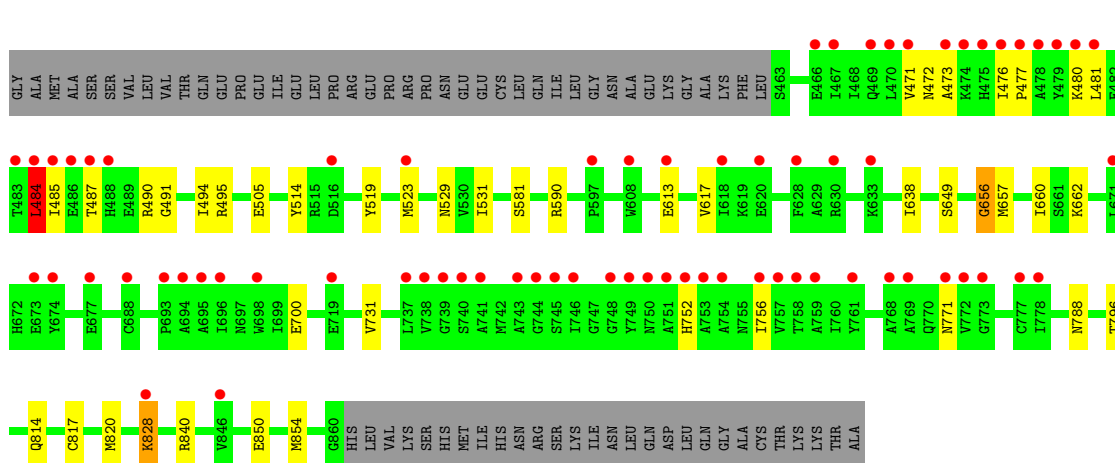
• Molecule 1: HMG-COA REDUCTASE

Chain A:



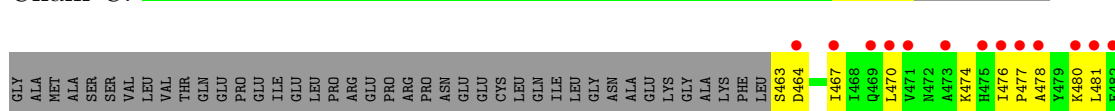
• Molecule 1: HMG-COA REDUCTASE

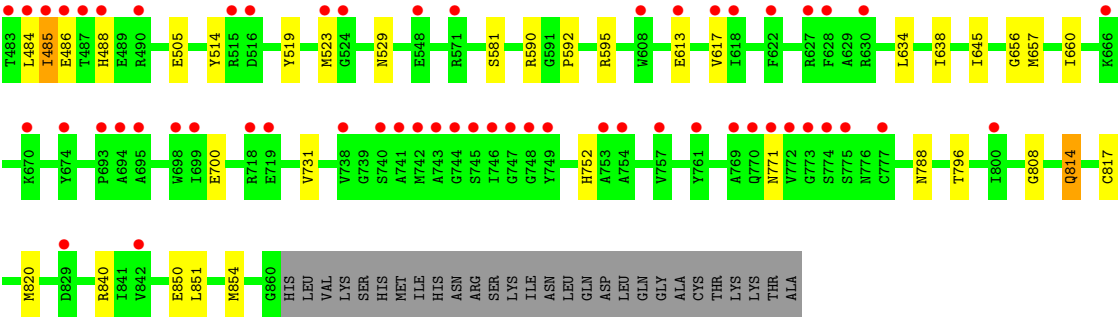
Chain B:



• Molecule 1: HMG-COA REDUCTASE

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.43Å 172.51Å 79.99Å 90.00° 117.36° 90.00°	Depositor
Resolution (Å)	43.29 – 2.10 43.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.29-2.10) 91.7 (43.29-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.239 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.2	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101827 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FBI, ADP

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	0.50	0/3072	0.67	0/4153
1	B	0.50	0/2994	0.67	1/4049 (0.0%)
1	C	0.49	0/2994	0.66	0/4049
1	D	0.54	0/2872	0.68	1/3882 (0.0%)
All	All	0.51	0/11932	0.67	2/16133 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	656	GLY	N-CA-C	5.30	126.34	113.10
1	B	656	GLY	N-CA-C	5.21	126.13	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3028	0	3059	29	0
1	B	2952	0	2989	33	0
1	C	2952	0	2989	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2832	0	2865	29	0
2	A	54	0	24	5	0
2	C	27	0	12	2	0
3	A	33	0	29	2	0
3	B	33	0	29	2	0
3	C	33	0	29	2	0
3	D	33	0	29	2	0
4	A	49	0	0	1	0
4	B	41	0	0	1	0
4	C	44	0	0	1	0
4	D	48	0	0	1	0
All	All	12159	0	12054	118	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 5.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:523:MET:HE1	4:D:1055:HOH:O	1.69	0.92
1:A:828:LYS:H	1:A:828:LYS:HD2	1.40	0.85
1:B:828:LYS:H	1:B:828:LYS:HD2	1.41	0.85
1:C:485:ILE:HG22	1:C:486:GLU:H	1.44	0.82
1:A:817:CYS:HA	1:A:820:MET:HE3	1.66	0.77
1:C:817:CYS:HA	1:C:820:MET:HE3	1.66	0.77
1:B:817:CYS:HA	1:B:820:MET:HE3	1.67	0.77
1:D:817:CYS:HA	1:D:820:MET:HE3	1.66	0.76
1:A:523:MET:HE1	4:A:1092:HOH:O	1.87	0.75
3:D:3:FBI:H91	3:D:3:FBI:H61	1.69	0.74
3:B:1:FBI:H61	3:B:1:FBI:H91	1.74	0.70
1:A:629:ALA:O	1:A:630:ARG:HD2	1.92	0.69
2:A:102:ADP:H2	1:B:529:ASN:HD22	1.39	0.68
1:B:828:LYS:H	1:B:828:LYS:CD	2.06	0.68
1:C:485:ILE:HG22	1:C:486:GLU:N	2.07	0.68
1:A:828:LYS:H	1:A:828:LYS:CD	2.07	0.68
1:B:523:MET:HE1	4:B:1108:HOH:O	1.95	0.64
2:A:102:ADP:H2	1:B:529:ASN:ND2	1.95	0.63
1:A:485:ILE:HD13	1:A:494:ILE:HD12	1.80	0.63
1:C:523:MET:HE1	4:C:1087:HOH:O	1.99	0.62
1:D:480:LYS:H	1:D:480:LYS:HD3	1.65	0.62
3:A:2:FBI:H61	3:A:2:FBI:H91	1.81	0.62
1:C:519:TYR:O	1:C:523:MET:HG2	2.00	0.62
1:D:519:TYR:O	1:D:523:MET:HG2	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:519:TYR:O	1:B:523:MET:HG2	2.02	0.60
1:A:519:TYR:O	1:A:523:MET:HG2	2.03	0.59
1:D:485:ILE:HG22	1:D:486:GLU:N	2.18	0.58
1:C:529:ASN:HD22	2:C:103:ADP:H2	1.52	0.58
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.85	0.58
3:A:2:FBI:H72	3:A:2:FBI:C86	2.34	0.57
1:C:485:ILE:CG2	1:C:486:GLU:H	2.17	0.56
1:D:656:GLY:O	1:D:660:ILE:HG12	2.06	0.56
1:D:581:SER:OG	1:D:840:ARG:HD2	2.07	0.55
1:C:529:ASN:ND2	2:C:103:ADP:H2	2.05	0.54
1:C:656:GLY:O	1:C:660:ILE:HG12	2.07	0.54
1:C:581:SER:OG	1:C:840:ARG:HD2	2.08	0.54
1:A:529:ASN:ND2	2:A:101:ADP:H2	2.05	0.54
1:D:523:MET:HE3	1:D:523:MET:HA	1.89	0.54
1:A:581:SER:OG	1:A:840:ARG:HD2	2.08	0.54
1:A:771:ASN:OD1	1:B:771:ASN:ND2	2.41	0.54
1:B:476:ILE:HD13	1:B:484:LEU:HD23	1.90	0.53
3:D:3:FBI:C86	3:D:3:FBI:H72	2.38	0.53
2:A:102:ADP:C2	1:B:529:ASN:ND2	2.77	0.53
1:C:771:ASN:OD1	1:D:771:ASN:ND2	2.42	0.52
1:A:771:ASN:ND2	1:B:771:ASN:OD1	2.43	0.52
1:C:477:PRO:HD2	1:C:480:LYS:HD2	1.92	0.52
1:B:581:SER:OG	1:B:840:ARG:HD2	2.09	0.52
1:A:485:ILE:CD1	1:A:494:ILE:HD12	2.40	0.51
1:B:485:ILE:HG22	1:B:487:THR:H	1.74	0.51
1:A:479:TYR:HA	1:A:495:ARG:NH1	2.26	0.51
1:B:656:GLY:O	1:B:660:ILE:HG12	2.10	0.51
1:B:487:THR:HG23	1:B:490:ARG:CB	2.41	0.50
1:C:771:ASN:ND2	1:D:771:ASN:OD1	2.44	0.49
1:B:796:THR:HG21	1:C:638:ILE:O	2.13	0.49
1:B:613:GLU:O	1:B:617:VAL:HG23	2.13	0.49
1:C:485:ILE:CG2	1:C:486:GLU:N	2.76	0.48
1:D:479:TYR:HA	1:D:495:ARG:NH1	2.28	0.48
1:B:485:ILE:CD1	1:B:494:ILE:HD12	2.44	0.47
1:D:731:VAL:HG12	1:D:854:MET:CE	2.44	0.47
3:C:4:FBI:H123	1:D:856:ALA:HB1	1.96	0.47
1:B:471:VAL:C	1:B:473:ALA:H	2.17	0.47
1:C:731:VAL:HG12	1:C:854:MET:CE	2.44	0.47
3:B:1:FBI:H72	3:B:1:FBI:C86	2.45	0.47
1:A:529:ASN:HD22	2:A:101:ADP:H2	1.61	0.47
1:A:613:GLU:O	1:A:617:VAL:HG23	2.15	0.47
1:C:613:GLU:O	1:C:617:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:463:SER:O	1:C:467:ILE:HG12	2.15	0.47
1:C:820:MET:HB2	1:C:820:MET:HE2	1.80	0.46
1:A:627:ARG:HH11	1:A:627:ARG:HG2	1.79	0.46
1:C:478:ALA:O	1:C:481:LEU:HG	2.16	0.46
1:A:477:PRO:HD2	1:A:480:LYS:HD2	1.97	0.46
1:B:731:VAL:HG12	1:B:854:MET:CE	2.46	0.46
1:A:638:ILE:O	1:D:796:THR:HG21	2.15	0.45
1:D:774:SER:HA	1:D:799:SER:O	2.17	0.45
1:A:731:VAL:HG12	1:A:854:MET:CE	2.46	0.45
1:A:629:ALA:C	1:A:630:ARG:HD2	2.37	0.45
1:B:481:LEU:HD12	1:B:495:ARG:HB2	1.99	0.45
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.84	0.45
1:D:485:ILE:HG22	1:D:486:GLU:H	1.83	0.44
1:D:649:SER:HB3	1:D:660:ILE:HD12	1.98	0.44
1:A:656:GLY:O	1:A:660:ILE:HG12	2.17	0.44
1:A:490:ARG:HD3	1:A:490:ARG:HA	1.73	0.44
1:D:485:ILE:CD1	1:D:494:ILE:HD12	2.48	0.43
1:D:523:MET:HA	1:D:523:MET:CE	2.48	0.43
1:D:820:MET:HB2	1:D:820:MET:HE2	1.81	0.43
1:C:592:PRO:HD2	1:C:645:ILE:O	2.17	0.43
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.84	0.43
1:C:481:LEU:O	1:C:485:ILE:HD12	2.19	0.43
1:D:485:ILE:CG2	1:D:486:GLU:N	2.81	0.43
1:D:662:LYS:HB3	1:D:662:LYS:HE2	1.83	0.42
1:C:488:HIS:CD2	1:C:523:MET:HG3	2.54	0.42
1:B:638:ILE:O	1:C:796:THR:HG21	2.19	0.42
1:B:484:LEU:HA	1:B:484:LEU:HD12	1.89	0.42
1:A:649:SER:HB3	1:A:660:ILE:HD12	2.02	0.42
1:D:592:PRO:HD2	1:D:645:ILE:O	2.20	0.42
1:C:731:VAL:HG12	1:C:854:MET:HE1	2.01	0.42
1:C:595:ARG:HH22	1:D:730:GLU:HG2	1.84	0.42
1:B:477:PRO:HD2	1:B:480:LYS:HD2	2.01	0.42
1:B:485:ILE:HD12	1:B:491:GLY:HA2	2.01	0.42
1:C:808:GLY:O	1:C:814:GLN:HG3	2.20	0.42
1:D:850:GLU:O	1:D:854:MET:HG2	2.19	0.42
1:A:796:THR:HG21	1:D:638:ILE:O	2.20	0.42
1:B:523:MET:HE3	1:B:523:MET:HA	2.01	0.41
1:A:461:PHE:HB3	1:A:462:LEU:HD12	2.03	0.41
1:C:850:GLU:O	1:C:854:MET:HG2	2.21	0.41
1:B:756:ILE:HD12	1:B:756:ILE:N	2.35	0.41
1:A:523:MET:HA	1:A:523:MET:CE	2.51	0.41
1:A:540:VAL:CG2	1:B:531:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:618:ILE:HG23	1:D:667:ALA:HB1	2.03	0.41
1:B:662:LYS:HB3	1:B:662:LYS:HE2	1.84	0.41
1:B:649:SER:HB3	1:B:660:ILE:HD12	2.03	0.40
3:C:4:FBI:H3	3:C:4:FBI:H62	1.89	0.40
1:B:850:GLU:O	1:B:854:MET:HG2	2.22	0.40
1:C:474:LYS:HB2	1:C:476:ILE:HG13	2.04	0.40
1:D:808:GLY:O	1:D:814:GLN:HG3	2.21	0.40
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.80	0.40
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.82	0.40
1:A:774:SER:HA	1:A:799:SER:O	2.21	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	403/467 (86%)	385 (96%)	15 (4%)	3 (1%)	30	23
1	B	396/467 (85%)	376 (95%)	17 (4%)	3 (1%)	27	20
1	C	396/467 (85%)	378 (96%)	16 (4%)	2 (0%)	38	33
1	D	380/467 (81%)	364 (96%)	15 (4%)	1 (0%)	50	49
All	All	1575/1868 (84%)	1503 (95%)	63 (4%)	9 (1%)	33	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	472	ASN
1	B	484	LEU
1	A	484	LEU
1	A	486	GLU
1	D	514	TYR
1	A	514	TYR
1	B	514	TYR
1	C	514	TYR

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Mol	Chain	Res	Type
1	C	485	ILE

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	325/375 (87%)	311 (96%)	14 (4%)	40	37
1	B	316/375 (84%)	308 (98%)	8 (2%)	60	63
1	C	316/375 (84%)	305 (96%)	11 (4%)	48	48
1	D	303/375 (81%)	293 (97%)	10 (3%)	50	51
All	All	1260/1500 (84%)	1217 (97%)	43 (3%)	49	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	LEU
1	A	484	LEU
1	A	486	GLU
1	A	505	GLU
1	A	627	ARG
1	A	634	LEU
1	A	657	MET
1	A	688	CYS
1	A	700	GLU
1	A	752	HIS
1	A	788	ASN
1	A	814	GLN
1	A	828	LYS
1	A	851	LEU
1	B	484	LEU
1	B	505	GLU
1	B	657	MET
1	B	700	GLU
1	B	752	HIS
1	B	788	ASN
1	B	814	GLN

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Mol	Chain	Res	Type
1	B	828	LYS
1	C	464	ASP
1	C	470	LEU
1	C	484	LEU
1	C	505	GLU
1	C	634	LEU
1	C	657	MET
1	C	700	GLU
1	C	752	HIS
1	C	788	ASN
1	C	814	GLN
1	C	851	LEU
1	D	480	LYS
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	700	GLU
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN
1	D	828	LYS
1	D	851	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	A	788	ASN
1	B	529	ASN
1	B	788	ASN
1	C	469	GLN
1	C	488	HIS
1	C	529	ASN
1	C	788	ASN
1	D	488	HIS
1	D	497	GLN
1	D	788	ASN
1	D	830	ASN

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 ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	101	-	29,29,29	1.33	4 (13%)	45,45,45	0.78	0
2	ADP	A	102	-	29,29,29	1.37	3 (10%)	45,45,45	0.86	1 (2%)
3	FBI	A	2	-	34,34,34	4.35	10 (29%)	49,49,49	2.22	14 (28%)
3	FBI	B	1	-	34,34,34	4.17	11 (32%)	49,49,49	2.30	14 (28%)
2	ADP	C	103	-	29,29,29	1.39	5 (17%)	45,45,45	1.03	3 (6%)
3	FBI	C	4	-	34,34,34	4.30	13 (38%)	49,49,49	2.32	14 (28%)
3	FBI	D	3	-	34,34,34	4.20	11 (32%)	49,49,49	2.25	14 (28%)

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
2	ADP	A	101	-	-	0/16/32/32	0/1/3/3
2	ADP	A	102	-	-	0/16/32/32	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBI	A	2	-	-	0/31/31/31	0/2/2/2
3	FBI	B	1	-	-	0/31/31/31	0/2/2/2
2	ADP	C	103	-	-	0/16/32/32	0/1/3/3
3	FBI	C	4	-	-	0/31/31/31	0/2/2/2
3	FBI	D	3	-	-	0/31/31/31	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	FBI	O1S-S1	15.47	1.60	1.43
3	C	4	FBI	O1S-S1	15.25	1.60	1.43
3	D	3	FBI	O2S-S1	14.49	1.59	1.43
3	A	2	FBI	O2S-S1	14.48	1.59	1.43
3	D	3	FBI	O1S-S1	14.40	1.59	1.43
3	B	1	FBI	O1S-S1	14.28	1.59	1.43
3	B	1	FBI	O2S-S1	14.02	1.59	1.43
3	C	4	FBI	O2S-S1	14.00	1.59	1.43
3	C	4	FBI	C81-C8	-9.10	1.38	1.48
3	B	1	FBI	C81-C8	-8.65	1.39	1.48
3	D	3	FBI	C81-C8	-8.56	1.39	1.48
3	A	2	FBI	C81-C8	-8.53	1.39	1.48
3	D	3	FBI	C9-C91	4.48	1.57	1.51
3	A	2	FBI	C11-N3	4.37	1.48	1.37
3	C	4	FBI	C6-C7	-4.04	1.32	1.53
3	A	2	FBI	C9-C91	3.95	1.56	1.51
3	D	3	FBI	C6-C7	-3.92	1.33	1.53
3	A	2	FBI	S1-N3	3.91	1.74	1.64
3	C	4	FBI	C9-C91	3.91	1.56	1.51
3	C	4	FBI	O1A-C1	3.88	1.36	1.22
3	B	1	FBI	O1A-C1	3.79	1.35	1.22
3	A	2	FBI	C6-C7	-3.78	1.33	1.53
3	D	3	FBI	O1A-C1	3.76	1.35	1.22
3	B	1	FBI	C6-C7	-3.76	1.33	1.53
3	D	3	FBI	S1-N3	3.75	1.74	1.64
3	C	4	FBI	C11-N3	3.71	1.46	1.37
3	B	1	FBI	C9-C91	3.70	1.56	1.51
3	B	1	FBI	C8-C10	3.68	1.45	1.41
3	C	4	FBI	S1-N3	3.63	1.74	1.64
3	B	1	FBI	C11-N3	3.48	1.46	1.37
2	C	103	ADP	C8-N7	-3.42	1.27	1.34
3	A	2	FBI	C8-C10	3.36	1.45	1.41
2	A	102	ADP	C8-N7	-3.16	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	ADP	C8-N7	-3.15	1.28	1.34
3	D	3	FBI	C11-N3	3.11	1.45	1.37
2	A	102	ADP	PA-O3A	3.06	1.65	1.59
3	B	1	FBI	S1-N3	2.97	1.72	1.64
3	A	2	FBI	O1B-C1	-2.90	1.20	1.30
2	C	103	ADP	C8-N9	-2.84	1.32	1.36
3	A	2	FBI	O1A-C1	2.82	1.32	1.22
2	A	101	ADP	C8-N9	-2.79	1.32	1.36
3	D	3	FBI	C10-C9	2.78	1.45	1.41
2	A	101	ADP	O4'-C4'	2.46	1.50	1.45
3	D	3	FBI	C8-C10	2.45	1.44	1.41
3	B	1	FBI	O1B-C1	-2.40	1.21	1.30
3	C	4	FBI	C8-C10	2.40	1.44	1.41
2	A	102	ADP	C8-N9	-2.38	1.33	1.36
3	C	4	FBI	C7-C10	2.23	1.55	1.52
2	A	101	ADP	PA-O3A	2.21	1.63	1.59
3	C	4	FBI	O1B-C1	-2.21	1.22	1.30
2	C	103	ADP	PB-O3A	-2.21	1.56	1.60
3	C	4	FBI	C11-N2	-2.18	1.30	1.34
3	B	1	FBI	C83-C84	2.16	1.41	1.36
3	D	3	FBI	O1B-C1	-2.15	1.22	1.30
2	C	103	ADP	C2'-C3'	2.14	1.59	1.53
2	C	103	ADP	O4'-C4'	2.13	1.50	1.45
3	C	4	FBI	C83-C84	2.11	1.41	1.36

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	FBI	O2S-S1-O1S	-8.47	106.86	118.68
3	C	4	FBI	O2S-S1-O1S	-8.44	106.90	118.68
3	A	2	FBI	O2S-S1-O1S	-7.66	107.98	118.68
3	D	3	FBI	O2S-S1-O1S	-7.52	108.18	118.68
3	D	3	FBI	O1S-S1-N3	5.63	113.39	107.07
3	B	1	FBI	C12-N3-C11	5.21	125.14	117.70
3	B	1	FBI	C6-C7-C10	5.09	128.02	112.28
3	D	3	FBI	C10-C9-N2	-4.87	118.90	123.19
3	C	4	FBI	C7-C6-C5	4.60	124.93	115.40
3	A	2	FBI	O2S-S1-N3	4.55	112.18	107.07
3	A	2	FBI	C6-C7-C10	4.53	126.31	112.28
3	A	2	FBI	C10-C9-N2	-4.53	119.20	123.19
3	D	3	FBI	C6-C7-C10	4.47	126.10	112.28
3	B	1	FBI	C10-C9-N2	-4.46	119.27	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	FBI	C12-N3-C11	4.37	123.94	117.70
3	A	2	FBI	C12-N3-C11	4.35	123.91	117.70
3	C	4	FBI	C6-C7-C10	4.29	125.54	112.28
3	B	1	FBI	O2S-S1-N3	4.14	111.72	107.07
3	C	4	FBI	C12-N3-C11	4.09	123.55	117.70
3	C	4	FBI	C10-C9-N2	-3.85	119.81	123.19
3	C	4	FBI	O1S-S1-N3	3.84	111.38	107.07
3	B	1	FBI	O1S-S1-N3	3.70	111.22	107.07
3	C	4	FBI	C8-N1-C11	3.66	120.67	115.92
3	A	2	FBI	C7-C6-C5	3.64	122.94	115.40
3	C	4	FBI	O2S-S1-N3	3.59	111.10	107.07
3	D	3	FBI	C7-C6-C5	3.53	122.70	115.40
3	A	2	FBI	C8-N1-C11	3.43	120.38	115.92
3	C	4	FBI	C10-C8-N1	-3.37	118.50	122.89
3	B	1	FBI	C7-C6-C5	3.28	122.19	115.40
3	D	3	FBI	C8-N1-C11	3.28	120.18	115.92
3	C	4	FBI	C13-S1-N3	3.13	110.57	105.95
3	B	1	FBI	C10-C8-N1	-3.11	118.85	122.89
3	D	3	FBI	C10-C8-N1	-3.02	118.97	122.89
3	B	1	FBI	C8-N1-C11	2.99	119.80	115.92
3	A	2	FBI	O1S-S1-N3	2.98	110.42	107.07
2	C	103	ADP	C4'-O4'-C1'	2.96	112.96	109.75
3	C	4	FBI	O1A-C1-C2	-2.95	112.15	122.62
3	B	1	FBI	C11-N2-C9	2.94	120.62	116.75
3	A	2	FBI	C10-C8-N1	-2.92	119.09	122.89
3	A	2	FBI	O1B-C1-C2	2.89	124.19	114.20
3	D	3	FBI	O1B-C1-C2	2.88	124.16	114.20
3	D	3	FBI	O1A-C1-C2	-2.88	112.42	122.62
3	A	2	FBI	C11-N2-C9	2.84	120.49	116.75
3	C	4	FBI	O1B-C1-C2	2.83	123.97	114.20
2	A	102	ADP	O4'-C1'-N9	-2.77	105.87	108.44
3	D	3	FBI	C13-S1-N3	2.73	109.97	105.95
3	A	2	FBI	C13-S1-N3	2.67	109.89	105.95
3	A	2	FBI	O1A-C1-C2	-2.63	113.28	122.62
3	B	1	FBI	O1B-C1-C2	2.63	123.27	114.20
3	C	4	FBI	C82-C81-C8	2.54	124.43	120.56
3	B	1	FBI	O1A-C1-C2	-2.51	113.72	122.62
3	D	3	FBI	C11-N2-C9	2.50	120.05	116.75
3	D	3	FBI	O2S-S1-N3	2.46	109.83	107.07
2	C	103	ADP	C3'-C2'-C1'	2.44	104.73	100.91
3	C	4	FBI	C11-N2-C9	2.42	119.94	116.75
2	C	103	ADP	C2'-C3'-C4'	2.25	107.14	102.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	FBI	C92-C91-C9	2.14	115.11	111.28
3	A	2	FBI	C91-C9-N2	2.12	117.51	115.73
3	B	1	FBI	C13-S1-N3	2.12	109.07	105.95
3	B	1	FBI	C3-C2-C1	2.01	116.96	112.90

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	407/467 (87%)	0.88	70 (17%) 2 2	35, 52, 90, 97	0
1	B	398/467 (85%)	0.89	71 (17%) 2 2	35, 52, 82, 100	0
1	C	398/467 (85%)	0.86	70 (17%) 2 2	36, 54, 89, 99	0
1	D	382/467 (81%)	0.71	46 (12%) 5 6	35, 50, 75, 100	0
All	All	1585/1868 (84%)	0.84	257 (16%) 2 2	35, 52, 87, 100	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	9.7
1	A	484	LEU	8.3
1	D	484	LEU	8.1
1	D	485	ILE	7.2
1	A	473	ALA	7.2
1	D	479	TYR	6.5
1	A	476	ILE	6.4
1	C	485	ILE	6.2
1	C	475	HIS	6.1
1	B	481	LEU	5.8
1	A	471	VAL	5.7
1	A	475	HIS	5.7
1	D	486	GLU	5.5
1	C	483	THR	5.3
1	C	471	VAL	5.2
1	B	484	LEU	5.2
1	A	772	VAL	5.2
1	B	486	GLU	5.1
1	B	485	ILE	5.1
1	C	484	LEU	5.1
1	D	746	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	471	VAL	5.0
1	D	481	LEU	4.9
1	B	478	ALA	4.9
1	D	694	ALA	4.8
1	B	476	ILE	4.8
1	B	475	HIS	4.7
1	C	486	GLU	4.7
1	C	470	LEU	4.6
1	A	483	THR	4.6
1	B	477	PRO	4.6
1	B	470	LEU	4.5
1	D	627	ARG	4.4
1	B	469	GLN	4.4
1	A	746	ILE	4.4
1	A	470	LEU	4.2
1	B	746	ILE	4.2
1	B	630	ARG	4.1
1	A	467	ILE	4.1
1	C	674	TYR	4.1
1	A	694	ALA	4.1
1	D	772	VAL	4.0
1	D	516	ASP	3.9
1	D	524	GLY	3.9
1	C	473	ALA	3.9
1	A	446	GLU	3.9
1	B	694	ALA	3.9
1	C	627	ARG	3.9
1	B	516	ASP	3.8
1	A	448	CYS	3.8
1	B	693	PRO	3.7
1	C	694	ALA	3.7
1	B	479	TYR	3.7
1	A	481	LEU	3.7
1	A	479	TYR	3.6
1	C	628	PHE	3.6
1	C	772	VAL	3.6
1	D	695	ALA	3.6
1	D	482	GLU	3.6
1	A	461	PHE	3.5
1	B	757	VAL	3.5
1	C	487	THR	3.5
1	A	699	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	523	MET	3.5
1	B	749	TYR	3.5
1	B	487	THR	3.5
1	D	745	SER	3.5
1	C	467	ILE	3.5
1	C	476	ILE	3.5
1	C	757	VAL	3.5
1	D	523	MET	3.4
1	C	741	ALA	3.4
1	D	743	ALA	3.4
1	B	467	ILE	3.4
1	B	754	ALA	3.4
1	B	620	GLU	3.3
1	C	695	ALA	3.3
1	A	769	ALA	3.3
1	C	745	SER	3.3
1	A	744	GLY	3.3
1	D	699	ILE	3.3
1	A	466	GLU	3.3
1	A	501	LYS	3.2
1	D	511	TYR	3.2
1	C	515	ARG	3.2
1	B	741	ALA	3.2
1	C	608	TRP	3.2
1	D	747	GLY	3.2
1	B	698	TRP	3.2
1	C	746	ILE	3.1
1	B	748	GLY	3.1
1	C	773	GLY	3.1
1	A	777	CYS	3.1
1	C	477	PRO	3.1
1	C	753	ALA	3.1
1	B	756	ILE	3.1
1	C	740	SER	3.1
1	C	769	ALA	3.1
1	B	758	THR	3.1
1	B	772	VAL	3.1
1	C	524	GLY	3.1
1	A	627	ARG	3.0
1	A	741	ALA	3.0
1	B	777	CYS	3.0
1	A	698	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	462	LEU	3.0
1	B	613	GLU	3.0
1	C	666	LYS	3.0
1	C	482	GLU	3.0
1	B	740	SER	3.0
1	A	745	SER	3.0
1	A	828	LYS	2.9
1	C	488	HIS	2.9
1	A	474	LYS	2.9
1	A	524	GLY	2.9
1	D	744	GLY	2.9
1	A	443	ARG	2.9
1	D	696	ILE	2.9
1	D	630	ARG	2.9
1	D	828	LYS	2.9
1	C	743	ALA	2.9
1	A	748	GLY	2.9
1	D	490	ARG	2.9
1	D	693	PRO	2.9
1	B	778	ILE	2.8
1	A	760	ILE	2.8
1	A	630	ARG	2.8
1	A	447	GLU	2.8
1	A	486	GLU	2.8
1	C	699	ILE	2.8
1	C	698	TRP	2.8
1	A	689	THR	2.8
1	B	474	LYS	2.8
1	B	695	ALA	2.8
1	B	743	ALA	2.8
1	A	693	PRO	2.8
1	A	786	PRO	2.7
1	B	473	ALA	2.7
1	D	515	ARG	2.7
1	C	481	LEU	2.7
1	A	695	ALA	2.7
1	C	718	ARG	2.7
1	D	748	GLY	2.7
1	D	758	THR	2.7
1	A	778	ILE	2.7
1	C	490	ARG	2.7
1	C	478	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	483	THR	2.6
1	D	487	THR	2.6
1	A	672	HIS	2.6
1	B	769	ALA	2.6
1	B	628	PHE	2.6
1	B	674	TYR	2.6
1	C	749	TYR	2.6
1	A	771	ASN	2.6
1	D	829	ASP	2.6
1	C	693	PRO	2.6
1	A	773	GLY	2.6
1	A	749	TYR	2.6
1	A	575	LEU	2.6
1	A	754	ALA	2.6
1	A	830	ASN	2.6
1	C	670	LYS	2.6
1	C	548	GLU	2.6
1	D	753	ALA	2.5
1	B	753	ALA	2.5
1	A	829	ASP	2.5
1	B	480	LYS	2.5
1	B	677	GLU	2.5
1	A	697	ASN	2.5
1	B	523	MET	2.5
1	C	761	TYR	2.5
1	B	738	VAL	2.5
1	B	745	SER	2.5
1	A	696	ILE	2.5
1	D	628	PHE	2.5
1	B	488	HIS	2.5
1	B	737	LEU	2.5
1	A	715	LYS	2.5
1	D	698	TRP	2.5
1	A	756	ILE	2.5
1	A	472	ASN	2.4
1	C	829	ASP	2.4
1	C	464	ASP	2.4
1	C	738	VAL	2.4
1	A	740	SER	2.4
1	C	516	ASP	2.4
1	C	754	ALA	2.4
1	B	828	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	740	SER	2.4
1	D	749	TYR	2.4
1	D	769	ALA	2.4
1	A	620	GLU	2.4
1	C	770	GLN	2.4
1	B	671	LEU	2.3
1	A	846	VAL	2.3
1	C	771	ASN	2.3
1	B	608	TRP	2.3
1	B	739	GLY	2.3
1	C	480	LYS	2.3
1	C	742	MET	2.3
1	A	747	GLY	2.3
1	C	630	ARG	2.3
1	A	480	LYS	2.3
1	D	778	ILE	2.3
1	C	747	GLY	2.3
1	C	617	VAL	2.3
1	D	757	VAL	2.3
1	C	775	SER	2.2
1	A	482	GLU	2.2
1	A	743	ALA	2.2
1	C	618	ILE	2.2
1	C	744	GLY	2.2
1	B	597	PRO	2.2
1	B	846	VAL	2.2
1	B	750	ASN	2.2
1	B	751	ALA	2.2
1	D	738	VAL	2.2
1	A	692	LYS	2.2
1	A	761	TYR	2.2
1	C	719	GLU	2.2
1	A	444	PRO	2.2
1	B	688	CYS	2.2
1	C	842	VAL	2.2
1	A	624	SER	2.2
1	D	775	SER	2.2
1	B	618	ILE	2.1
1	B	633	LYS	2.1
1	B	761	TYR	2.1
1	C	613	GLU	2.1
1	D	759	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	798	PRO	2.1
1	A	758	THR	2.1
1	B	673	GLU	2.1
1	B	744	GLY	2.1
1	B	773	GLY	2.1
1	D	773	GLY	2.1
1	C	469	GLN	2.1
1	A	485	ILE	2.1
1	B	696	ILE	2.1
1	D	737	LEU	2.1
1	B	768	ALA	2.1
1	C	800	ILE	2.1
1	B	771	ASN	2.1
1	C	774	SER	2.1
1	B	759	ALA	2.1
1	C	777	CYS	2.1
1	C	748	GLY	2.1
1	C	571	ARG	2.0
1	A	677	GLU	2.0
1	B	466	GLU	2.0
1	C	622	PHE	2.0
1	D	556	ALA	2.0
1	B	719	GLU	2.0
1	D	742	MET	2.0
1	B	752	HIS	2.0
1	A	688	CYS	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(\AA^2)	Q<0.9
2	ADP	C	103	27/27	0.27	1.31	83,88,99,99	0
2	ADP	A	102	27/27	0.24	0.60	88,91,99,99	0
2	ADP	A	101	27/27	0.24	0.59	90,93,99,99	0
3	FBI	D	3	33/33	0.13	-0.29	44,51,57,58	0
3	FBI	C	4	33/33	0.13	-0.34	44,51,57,57	0
3	FBI	B	1	33/33	0.12	-0.64	46,54,59,59	0
3	FBI	A	2	33/33	0.13	-0.66	41,48,52,53	0

6.5 Other polymers

There are no such residues in this entry.