



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:35 PM GMT

PDB ID : 1HWK  
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH ATORVASTATIN  
Authors : Istvan, E.S.; Deisenhofer, J.  
Deposited on : 2001-01-09  
Resolution : 2.22 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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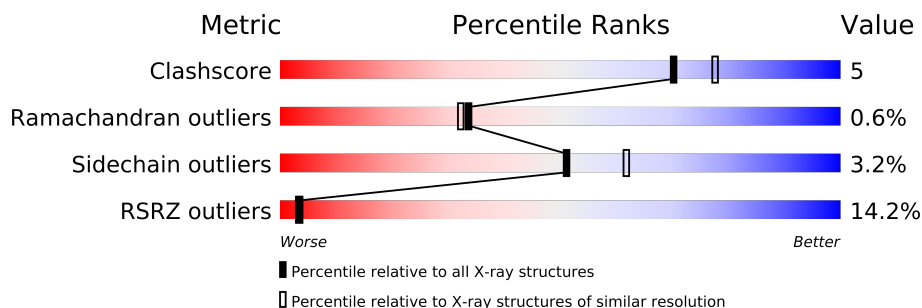
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.22 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	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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  $\geq 3$ , 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ADP	A	103	-	X
2	ADP	B	104	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12296 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	408	Total	C	N	O	S	0	0	0
			3035	1889	534	582	30			
1	B	393	Total	C	N	O	S	0	0	0
			2913	1812	510	562	29			
1	C	399	Total	C	N	O	S	0	0	0
			2960	1844	519	568	29			
1	D	387	Total	C	N	O	S	0	0	0
			2864	1779	502	554	29			

There are 20 discrepancies between the modelled and reference sequences:

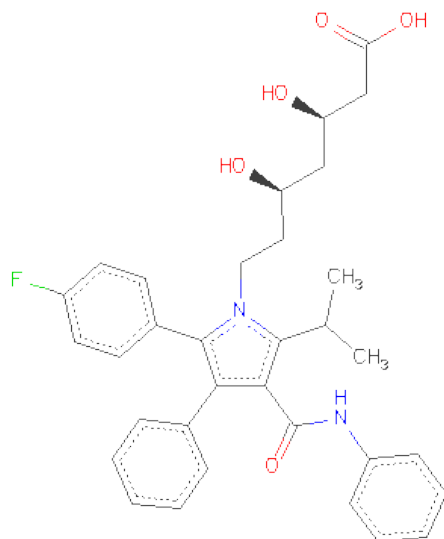
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	INSERTION	UNP P04035
A	423	ALA	-	INSERTION	UNP P04035
A	424	MET	-	INSERTION	UNP P04035
A	425	ALA	-	INSERTION	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	422	GLY	-	INSERTION	UNP P04035
B	423	ALA	-	INSERTION	UNP P04035
B	424	MET	-	INSERTION	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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]-3,5-DIHYDROXY-HEPTANOICACID (three-letter code: 117) (formula:  $C_{33}H_{35}FN_2O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	A	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	D	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	C	1	Total	C	F	N	O	0	0
			41	33	1	2	5		

- Molecule 4 is water.

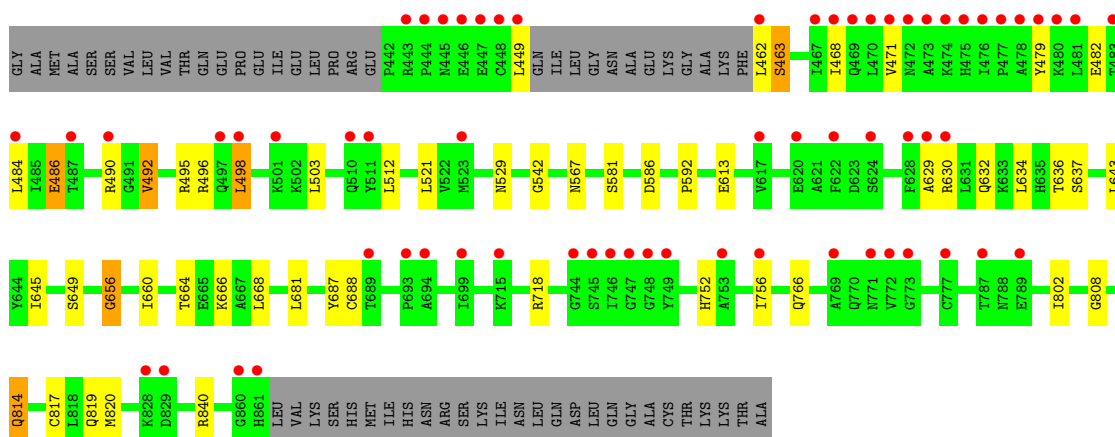
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	48	Total	O	0	0
			48	48		
4	C	57	Total	O	0	0
			57	57		
4	D	61	Total	O	0	0
			61	61		

### 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.

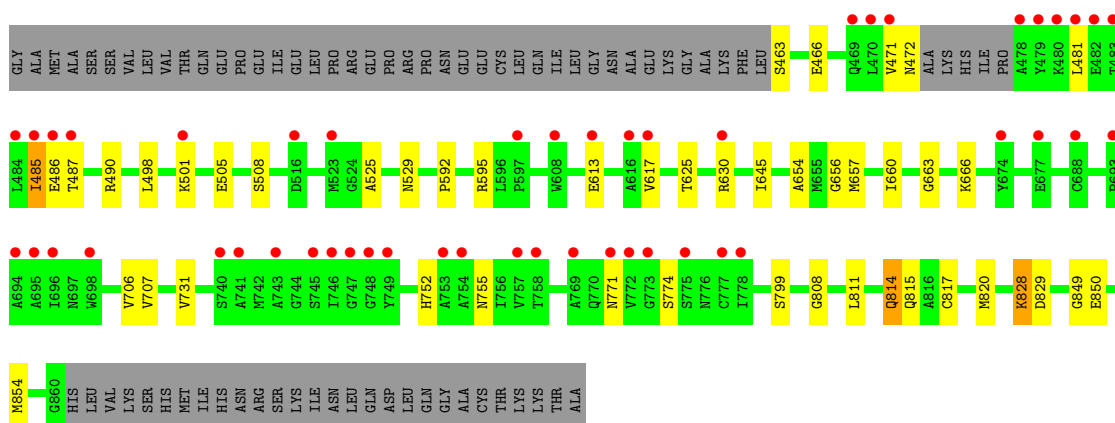
#### • Molecule 1: HMG-COA REDUCTASE

Chain A: 



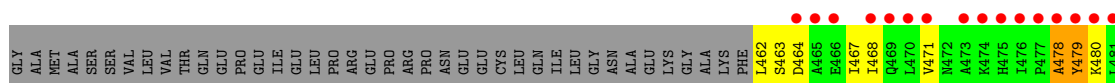
#### • Molecule 1: HMG-COA REDUCTASE

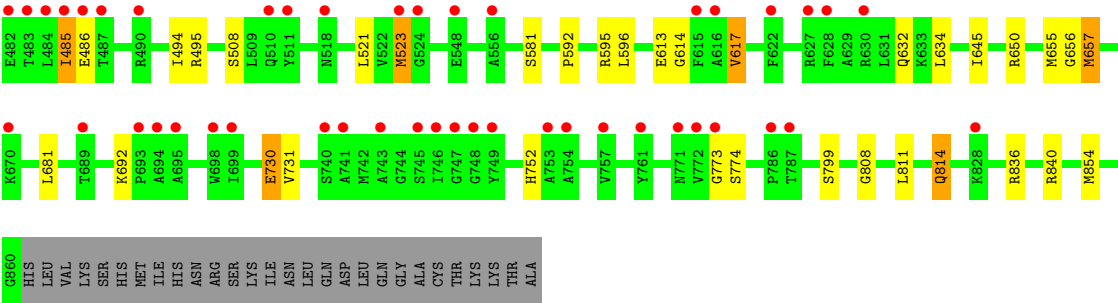
Chain B: 



#### • Molecule 1: HMG-COA REDUCTASE

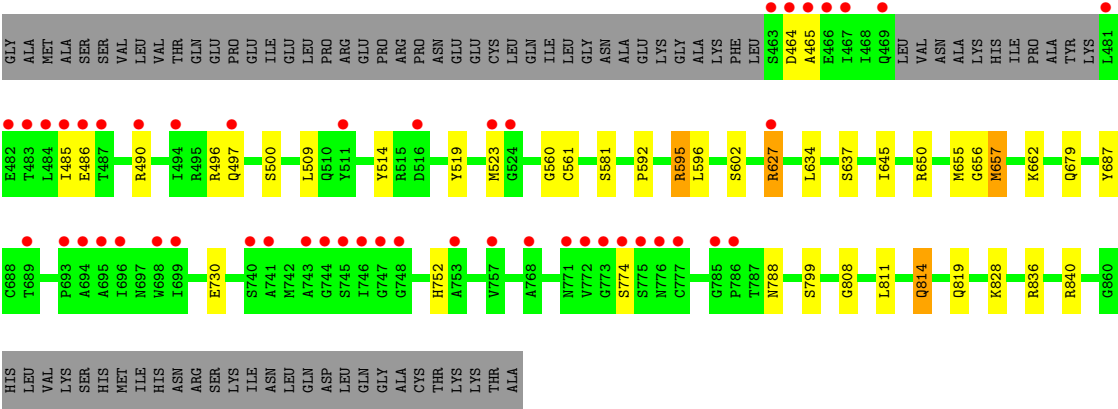
Chain C: 





• Molecule 1: HMG-COA REDUCTASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.60Å 172.72Å 80.01Å 90.00° 117.73° 90.00°	Depositor
Resolution (Å)	43.40 – 2.22 54.76 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.40-2.22) 93.0 (54.76-2.21)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.235 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.8	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 87319 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 117, 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	0.49	0/3079	0.67	1/4163 (0.0%)
1	B	0.48	0/2952	0.66	1/3990 (0.0%)
1	C	0.47	0/3002	0.65	2/4060 (0.0%)
1	D	0.51	0/2902	0.66	1/3922 (0.0%)
All	All	0.49	0/11935	0.66	5/16135 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	LEU	CA-CB-CG	-5.42	102.84	115.30
1	A	656	GLY	N-CA-C	5.28	126.29	113.10
1	D	656	GLY	N-CA-C	5.24	126.21	113.10
1	B	656	GLY	N-CA-C	5.21	126.12	113.10
1	C	656	GLY	N-CA-C	5.04	125.71	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	3035	0	3068	31	0
1	B	2913	0	2945	31	0
1	C	2960	0	3000	31	0
1	D	2864	0	2892	23	0
2	A	81	0	36	3	0
2	B	27	0	12	1	0
2	D	27	0	12	0	0
3	A	41	0	34	0	0
3	B	41	0	34	0	0
3	C	41	0	34	0	0
3	D	41	0	34	0	0
4	A	59	0	0	0	0
4	B	48	0	0	1	0
4	C	57	0	0	2	0
4	D	61	0	0	0	0
All	All	12296	0	12101	111	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 (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:625:THR:HG22	1:B:666:LYS:HD2	1.44	1.00
1:B:485:ILE:HG22	1:B:486:GLU:H	1.31	0.96
1:C:485:ILE:HG22	1:C:486:GLU:H	1.30	0.95
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.58	0.85
1:C:479:TYR:HA	1:C:495:ARG:HH11	1.47	0.80
1:A:542:GLY:H	1:A:567:ASN:ND2	1.78	0.79
1:B:752:HIS:HD2	1:B:755:ASN:HD22	1.30	0.79
1:C:632:GLN:HE21	1:C:650:ARG:HG3	1.52	0.74
1:C:479:TYR:HA	1:C:495:ARG:NH1	2.04	0.73
1:D:485:ILE:HG22	1:D:486:GLU:H	1.55	0.71
1:B:654:ALA:HB1	2:B:104:ADP:O1B	1.93	0.69
1:D:485:ILE:HG22	1:D:486:GLU:N	2.11	0.65
1:D:581:SER:OG	1:D:840:ARG:HD2	1.96	0.65
1:C:581:SER:OG	1:C:840:ARG:HD2	1.96	0.63
1:C:485:ILE:HG22	1:C:486:GLU:N	2.11	0.62
1:C:485:ILE:HD11	1:C:494:ILE:HD12	1.80	0.62
1:B:485:ILE:HG22	1:B:486:GLU:N	2.10	0.61
1:C:523:MET:HE1	4:C:1227:HOH:O	2.01	0.60
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.84	0.60
1:B:817:CYS:HA	1:B:820:MET:HE3	1.84	0.59
1:A:529:ASN:HD21	2:A:101:ADP:H2	1.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:613:GLU:O	1:C:617:VAL:HG12	2.04	0.58
1:A:462:LEU:O	1:A:463:SER:HB3	2.04	0.58
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.34	0.57
1:C:467:ILE:O	1:C:471:VAL:HG23	2.05	0.56
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.87	0.56
1:C:730:GLU:HG2	1:D:595:ARG:HH12	1.71	0.56
1:A:629:ALA:O	1:A:630:ARG:HD2	2.06	0.56
1:A:656:GLY:O	1:A:660:ILE:HG12	2.06	0.56
1:B:752:HIS:CD2	1:B:755:ASN:HD22	2.18	0.55
1:A:479:TYR:HB3	1:A:529:ASN:OD1	2.07	0.55
1:D:519:TYR:O	1:D:523:MET:HG2	2.07	0.55
1:C:808:GLY:O	1:C:814:GLN:HG3	2.08	0.54
1:D:808:GLY:O	1:D:814:GLN:HG3	2.07	0.54
1:C:464:ASP:O	1:C:468:ILE:HG12	2.07	0.54
1:C:463:SER:O	1:C:467:ILE:HG12	2.08	0.54
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.08	0.53
1:A:542:GLY:H	1:A:567:ASN:HD21	1.55	0.53
1:D:595:ARG:HD2	1:D:679:GLN:OE1	2.08	0.53
1:A:819:GLN:HB3	1:B:508:SER:CB	2.38	0.53
1:A:581:SER:OG	1:A:840:ARG:HD2	2.08	0.53
1:A:718:ARG:HG3	1:A:718:ARG:HH11	1.75	0.52
1:D:596:LEU:HD13	1:D:602:SER:HA	1.92	0.51
1:B:498:LEU:O	1:B:501:LYS:HG2	2.10	0.51
1:A:613:GLU:CD	1:A:613:GLU:H	2.14	0.51
1:B:752:HIS:HE1	1:B:849:GLY:O	1.94	0.50
1:A:819:GLN:HB3	1:B:508:SER:HB2	1.92	0.50
1:A:542:GLY:H	1:A:567:ASN:HD22	1.58	0.49
1:D:655:MET:SD	1:D:657:MET:HG2	2.52	0.48
1:A:808:GLY:O	1:A:814:GLN:HG3	2.12	0.48
1:A:492:VAL:O	1:A:496:ARG:HG2	2.14	0.48
1:B:811:LEU:O	1:B:815:GLN:HG3	2.14	0.47
1:B:808:GLY:O	1:B:814:GLN:HG3	2.15	0.47
1:B:481:LEU:HD22	1:B:481:LEU:H	1.78	0.47
1:A:649:SER:HB3	1:A:660:ILE:HD12	1.96	0.47
1:C:655:MET:SD	1:C:657:MET:HG2	2.55	0.46
1:B:828:LYS:HD2	1:B:829:ASP:H	1.81	0.46
1:D:485:ILE:CG2	1:D:486:GLU:H	2.25	0.46
1:B:471:VAL:O	1:B:472:ASN:HB2	2.16	0.45
1:D:485:ILE:CG2	1:D:486:GLU:N	2.80	0.45
1:D:662:LYS:HB3	1:D:662:LYS:HE2	1.77	0.45
1:B:731:VAL:HG12	1:B:854:MET:CE	2.46	0.45
1:B:811:LEU:HB2	1:B:814:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:706:VAL:HG12	1:B:707:VAL:N	2.32	0.45
1:A:817:CYS:HA	1:A:820:MET:HE3	2.00	0.44
1:C:478:ALA:O	1:C:480:LYS:N	2.47	0.44
1:A:586:ASP:O	1:A:632:GLN:NE2	2.45	0.44
1:C:692:LYS:HB2	1:C:692:LYS:HE2	1.86	0.44
1:C:523:MET:CE	1:C:523:MET:HA	2.48	0.44
1:B:595:ARG:HD3	4:B:1036:HOH:O	2.18	0.43
1:A:637:SER:HB2	1:A:687:TYR:OH	2.17	0.43
1:B:850:GLU:O	1:B:854:MET:HG2	2.18	0.43
1:C:462:LEU:HD12	1:C:462:LEU:N	2.33	0.43
1:A:484:LEU:HD23	1:A:484:LEU:O	2.19	0.43
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:C:508:SER:HB2	1:D:819:GLN:HB3	2.01	0.43
1:C:614:GLY:O	1:C:617:VAL:HG13	2.18	0.43
1:D:650:ARG:NH1	1:D:836:ARG:HH21	2.17	0.43
1:B:463:SER:OG	1:B:466:GLU:HG2	2.17	0.43
1:A:756:ILE:HD12	1:A:756:ILE:N	2.33	0.43
1:D:485:ILE:HG21	1:D:490:ARG:HD3	1.99	0.43
1:D:627:ARG:N	1:D:627:ARG:HD3	2.34	0.43
2:A:102:ADP:H2	1:B:529:ASN:HD21	1.66	0.42
1:C:773:GLY:HA3	4:C:1171:HOH:O	2.19	0.42
1:B:613:GLU:O	1:B:617:VAL:HG23	2.20	0.42
1:A:664:THR:O	1:A:668:LEU:HG	2.20	0.42
1:C:592:PRO:HD2	1:C:645:ILE:O	2.19	0.42
1:C:595:ARG:HD2	1:C:681:LEU:HD22	2.00	0.42
1:B:625:THR:HG21	1:B:663:GLY:HA2	2.00	0.42
1:A:529:ASN:ND2	2:A:101:ADP:H2	2.17	0.42
1:B:774:SER:HA	1:B:799:SER:O	2.20	0.42
1:C:478:ALA:C	1:C:480:LYS:H	2.22	0.41
1:B:592:PRO:HD2	1:B:645:ILE:O	2.19	0.41
1:A:479:TYR:HA	1:A:495:ARG:HH21	1.85	0.41
1:C:811:LEU:HB2	1:C:814:GLN:HG2	2.02	0.41
1:D:637:SER:HB2	1:D:687:TYR:OH	2.20	0.41
1:C:650:ARG:NH1	1:C:836:ARG:HH21	2.18	0.41
1:A:819:GLN:HB3	1:B:508:SER:HB3	2.01	0.41
1:C:731:VAL:HG12	1:C:854:MET:CE	2.51	0.41
1:D:592:PRO:HD2	1:D:645:ILE:O	2.21	0.41
1:D:496:ARG:NH2	1:D:509:LEU:O	2.54	0.41
1:C:774:SER:HA	1:C:799:SER:O	2.20	0.41
1:B:487:THR:HG23	1:B:490:ARG:CB	2.50	0.41
1:A:468:ILE:HG23	1:A:498:LEU:CD1	2.51	0.40
1:C:657:MET:HA	1:C:657:MET:CE	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:497:GLN:O	1:D:500:SER:HB3	2.21	0.40
1:C:467:ILE:HG21	1:C:494:ILE:HD13	2.02	0.40
1:D:811:LEU:HB2	1:D:814:GLN:HG2	2.04	0.40
1:B:731:VAL:HG12	1:B:854:MET:HE3	2.04	0.40
1:A:592:PRO:HD2	1:A:645:ILE:O	2.21	0.40
1:D:560:GLY:O	1:D:561:CYS:HB2	2.22	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	404/467 (86%)	385 (95%)	17 (4%)	2 (0%)	38	38
1	B	389/467 (83%)	372 (96%)	15 (4%)	2 (0%)	38	38
1	C	397/467 (85%)	382 (96%)	12 (3%)	3 (1%)	27	24
1	D	383/467 (82%)	366 (96%)	15 (4%)	2 (0%)	38	38
All	All	1573/1868 (84%)	1505 (96%)	59 (4%)	9 (1%)	33	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	C	478	ALA
1	C	479	TYR
1	D	465	ALA
1	B	525	ALA
1	D	514	TYR
1	A	463	SER
1	C	485	ILE
1	B	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	326/375 (87%)	311 (95%)	15 (5%)	37	43
1	B	312/375 (83%)	305 (98%)	7 (2%)	64	76
1	C	317/375 (84%)	309 (98%)	8 (2%)	60	71
1	D	307/375 (82%)	297 (97%)	10 (3%)	50	60
All	All	1262/1500 (84%)	1222 (97%)	40 (3%)	51	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	LEU
1	A	482	GLU
1	A	486	GLU
1	A	490	ARG
1	A	492	VAL
1	A	498	LEU
1	A	503	LEU
1	A	512	LEU
1	A	521	LEU
1	A	634	LEU
1	A	666	LYS
1	A	681	LEU
1	A	688	CYS
1	A	752	HIS
1	A	814	GLN
1	B	505	GLU
1	B	630	ARG
1	B	657	MET
1	B	660	ILE
1	B	771	ASN
1	B	814	GLN
1	B	828	LYS
1	C	521	LEU
1	C	523	MET
1	C	617	VAL
1	C	634	LEU

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Mol	Chain	Res	Type
1	C	657	MET
1	C	730	GLU
1	C	752	HIS
1	C	814	GLN
1	D	464	ASP
1	D	595	ARG
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	730	GLU
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN
1	D	828	LYS

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	445	ASN
1	A	469	GLN
1	A	567	ASN
1	A	814	GLN
1	B	632	GLN
1	B	635	HIS
1	B	752	HIS
1	C	469	GLN
1	C	819	GLN
1	D	488	HIS
1	D	788	ASN
1	D	819	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 ⓘ

9 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	1.36	4 (13%)	45,45,45	0.75	0
2	ADP	A	102	-	29,29,29	1.39	6 (20%)	45,45,45	0.92	2 (4%)
2	ADP	A	103	-	29,29,29	1.60	7 (24%)	45,45,45	1.36	3 (6%)
3	117	A	2	-	44,44,44	1.97	11 (25%)	60,61,61	1.44	11 (18%)
3	117	B	1	-	44,44,44	1.96	11 (25%)	60,61,61	1.47	10 (16%)
2	ADP	B	104	-	29,29,29	1.87	7 (24%)	45,45,45	0.99	1 (2%)
3	117	C	4	-	44,44,44	1.90	12 (27%)	60,61,61	1.48	10 (16%)
2	ADP	D	105	-	29,29,29	1.45	6 (20%)	45,45,45	0.90	1 (2%)
3	117	D	3	-	44,44,44	1.84	9 (20%)	60,61,61	1.44	10 (16%)

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
2	ADP	A	103	-	-	0/16/32/32	0/1/3/3
3	117	A	2	-	-	2/33/33/33	0/4/4/4
3	117	B	1	-	-	2/33/33/33	0/4/4/4
2	ADP	B	104	-	-	0/16/32/32	0/1/3/3
3	117	C	4	-	-	2/33/33/33	0/4/4/4
2	ADP	D	105	-	-	0/16/32/32	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	117	D	3	-	-	2/33/33/33	0/4/4/4

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	117	C19-N2	-7.30	1.27	1.41
3	B	1	117	C19-N2	-6.80	1.28	1.41
3	C	4	117	C19-N2	-6.59	1.28	1.41
3	D	3	117	C19-N2	-5.49	1.31	1.41
2	B	104	ADP	PA-O3A	5.42	1.69	1.59
3	D	3	117	C9-N1	4.46	1.41	1.36
3	B	1	117	C9-N1	4.29	1.41	1.36
3	C	4	117	C9-N1	4.05	1.40	1.36
3	A	2	117	C9-C91	4.01	1.58	1.51
3	B	1	117	C10-C12	-3.97	1.42	1.50
3	D	3	117	C10-C12	-3.89	1.42	1.50
3	D	3	117	C9-C91	3.62	1.57	1.51
2	A	103	ADP	PA-O3A	3.51	1.66	1.59
3	C	4	117	C9-C91	3.51	1.57	1.51
3	D	3	117	O1A-C1	3.48	1.34	1.22
3	B	1	117	O1A-C1	3.43	1.34	1.22
3	B	1	117	C18-N2	3.42	1.44	1.35
3	A	2	117	C11-C9	3.35	1.43	1.39
2	B	104	ADP	O4'-C1'	3.35	1.46	1.41
3	D	3	117	C18-N2	3.32	1.44	1.35
3	A	2	117	C9-N1	3.24	1.39	1.36
3	C	4	117	C18-N2	3.23	1.44	1.35
3	C	4	117	C10-C12	-3.20	1.43	1.50
3	C	4	117	O1A-C1	3.16	1.33	1.22
2	A	103	ADP	O4'-C4'	3.13	1.52	1.45
2	A	103	ADP	C8-N7	-3.09	1.28	1.34
2	D	105	ADP	PA-O3A	3.09	1.65	1.59
2	D	105	ADP	C8-N7	-3.08	1.28	1.34
2	A	101	ADP	C8-N7	-3.07	1.28	1.34
3	A	2	117	O1A-C1	3.06	1.33	1.22
2	B	104	ADP	C8-N7	-3.05	1.28	1.34
3	A	2	117	C10-C12	-3.02	1.44	1.50
3	B	1	117	C9-C91	3.01	1.56	1.51
2	B	104	ADP	O4'-C4'	2.98	1.52	1.45
2	A	102	ADP	PA-O3A	2.91	1.65	1.59
2	A	102	ADP	C8-N7	-2.89	1.28	1.34
2	A	101	ADP	PA-O3A	2.79	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	117	C11-C18	2.75	1.55	1.50
3	A	2	117	C18-N2	2.74	1.42	1.35
3	B	1	117	C83-C84	2.67	1.42	1.36
2	B	104	ADP	C8-N9	-2.62	1.32	1.36
3	C	4	117	C83-C84	2.61	1.42	1.36
3	A	2	117	C13-C12	2.55	1.44	1.39
2	D	105	ADP	C8-N9	-2.53	1.32	1.36
2	B	104	ADP	C2'-C3'	2.49	1.60	1.53
2	D	105	ADP	O4'-C4'	2.47	1.50	1.45
2	A	101	ADP	C8-N9	-2.45	1.33	1.36
2	A	103	ADP	O4'-C1'	2.40	1.45	1.41
3	C	4	117	C11-C9	2.39	1.41	1.39
3	A	2	117	O1B-C1	-2.37	1.21	1.30
2	A	103	ADP	C2'-C3'	2.36	1.60	1.53
3	C	4	117	C24-C19	2.35	1.43	1.39
2	A	101	ADP	O4'-C4'	2.35	1.50	1.45
3	B	1	117	C11-C9	2.33	1.41	1.39
2	A	102	ADP	C8-N9	-2.26	1.33	1.36
2	A	103	ADP	C8-N9	-2.21	1.33	1.36
3	B	1	117	O1B-C1	-2.19	1.22	1.30
3	A	2	117	C8-N1	2.16	1.43	1.40
2	A	102	ADP	C2'-C3'	2.15	1.59	1.53
2	B	104	ADP	C5-C4	-2.15	1.35	1.40
3	C	4	117	C81-C8	-2.14	1.41	1.48
2	A	102	ADP	O4'-C4'	2.13	1.50	1.45
3	D	3	117	C11-C9	2.11	1.41	1.39
3	C	4	117	O1B-C1	-2.10	1.22	1.30
3	C	4	117	C8-N1	2.08	1.43	1.40
2	A	103	ADP	C1'-N9	2.08	1.55	1.48
3	D	3	117	C24-C19	2.07	1.42	1.39
3	B	1	117	C11-C18	2.05	1.54	1.50
2	D	105	ADP	O4'-C1'	2.04	1.44	1.41
3	A	2	117	C81-C8	-2.02	1.42	1.48
2	D	105	ADP	C2'-C3'	2.01	1.59	1.53
3	B	1	117	C82-C83	2.01	1.42	1.38
2	A	102	ADP	C1'-N9	2.01	1.54	1.48

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	103	ADP	O4'-C1'-N9	6.95	114.90	108.44
3	C	4	117	C8-N1-C9	-5.74	104.77	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	117	C8-N1-C9	-5.26	105.11	108.81
3	A	2	117	C8-N1-C9	-4.91	105.36	108.81
3	D	3	117	C8-N1-C9	-4.29	105.79	108.81
3	B	1	117	C11-C9-N1	4.04	111.03	107.92
2	B	104	ADP	O4'-C1'-N9	3.85	112.02	108.44
3	C	4	117	C11-C9-N1	3.79	110.83	107.92
3	D	3	117	C7-C6-C5	-3.78	110.23	113.82
3	D	3	117	C11-C9-N1	3.49	110.60	107.92
2	D	105	ADP	O4'-C1'-N9	3.33	111.53	108.44
3	A	2	117	C11-C9-N1	3.22	110.40	107.92
3	B	1	117	C5-C4-C3	-3.17	110.15	114.65
3	D	3	117	C11-C18-N2	3.02	121.63	115.50
3	B	1	117	O1B-C1-C2	3.00	124.55	114.20
3	B	1	117	O1A-C1-C2	-2.95	112.15	122.62
3	C	4	117	O1A-C1-C2	-2.93	112.22	122.62
3	D	3	117	O1A-C1-C2	-2.92	112.26	122.62
3	A	2	117	C11-C18-N2	2.92	121.42	115.50
3	C	4	117	C10-C8-N1	2.82	111.01	108.24
3	C	4	117	O1B-C1-C2	2.80	123.89	114.20
3	D	3	117	O1B-C1-C2	2.73	123.62	114.20
3	D	3	117	C10-C8-N1	2.72	110.92	108.24
3	A	2	117	C10-C8-N1	2.72	110.91	108.24
2	A	102	ADP	C4'-O4'-C1'	2.70	112.68	109.75
3	A	2	117	O18-C18-C11	-2.67	116.71	120.79
3	B	1	117	C7-C6-C5	-2.67	111.28	113.82
3	A	2	117	O1A-C1-C2	-2.67	113.16	122.62
3	D	3	117	C10-C11-C18	2.61	131.21	126.31
3	A	2	117	O1B-C1-C2	2.56	123.05	114.20
3	C	4	117	C11-C18-N2	2.51	120.60	115.50
3	C	4	117	C7-N1-C8	2.42	128.66	124.83
2	A	102	ADP	C3'-C2'-C1'	2.27	104.46	100.91
3	A	2	117	C82-C81-C8	2.24	124.71	120.40
3	D	3	117	O18-C18-C11	-2.21	117.42	120.79
3	B	1	117	C82-C81-C8	2.21	124.65	120.40
3	B	1	117	C10-C8-N1	2.20	110.41	108.24
3	A	2	117	C7-N1-C8	2.18	128.28	124.83
3	C	4	117	C82-C81-C8	2.16	124.57	120.40
3	C	4	117	C10-C11-C18	2.15	130.35	126.31
3	C	4	117	O18-C18-C11	-2.11	117.57	120.79
3	B	1	117	C11-C18-N2	2.06	119.69	115.50
3	D	3	117	C82-C83-C84	2.04	120.49	118.33
2	A	103	ADP	C4'-O4'-C1'	2.03	111.95	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	103	ADP	C3'-C2'-C1'	2.02	104.07	100.91
3	A	2	117	C82-C83-C84	2.02	120.47	118.33
3	A	2	117	C10-C11-C18	2.01	130.08	126.31
3	B	1	117	C7-N1-C8	2.01	128.01	124.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	117	O18-C18-C11-C10
3	D	3	117	C10-C11-C18-N2
3	C	4	117	O18-C18-C11-C10
3	C	4	117	C10-C11-C18-N2
3	B	1	117	O18-C18-C11-C10
3	B	1	117	C10-C11-C18-N2
3	A	2	117	O18-C18-C11-C10
3	A	2	117	C10-C11-C18-N2

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	408/467 (87%)	0.79	64 (15%) 3 3	30, 48, 93, 100	0
1	B	393/467 (84%)	0.68	49 (12%) 5 4	30, 48, 77, 100	0
1	C	399/467 (85%)	0.84	61 (15%) 3 3	32, 50, 94, 100	0
1	D	387/467 (82%)	0.58	48 (12%) 5 4	30, 45, 75, 100	0
All	All	1587/1868 (84%)	0.72	222 (13%) 3 3	30, 48, 91, 100	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	10.7
1	D	483	THR	9.9
1	A	473	ALA	8.7
1	A	484	LEU	8.5
1	C	475	HIS	8.5
1	B	485	ILE	8.3
1	D	484	LEU	8.2
1	C	476	ILE	8.0
1	D	485	ILE	7.9
1	B	486	GLU	7.3
1	A	475	HIS	7.3
1	C	477	PRO	7.2
1	D	467	ILE	7.1
1	C	627	ARG	6.9
1	C	483	THR	6.8
1	B	487	THR	6.6
1	C	478	ALA	6.6
1	C	473	ALA	6.4
1	A	470	LEU	6.2
1	B	479	TYR	6.1
1	A	448	CYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	479	TYR	5.9
1	A	479	TYR	5.9
1	C	484	LEU	5.8
1	A	449	LEU	5.8
1	C	628	PHE	5.7
1	D	466	GLU	5.7
1	C	486	GLU	5.5
1	D	486	GLU	5.5
1	A	861	HIS	5.4
1	B	483	THR	5.4
1	B	478	ALA	5.4
1	D	481	LEU	5.2
1	D	487	THR	5.2
1	C	470	LEU	5.2
1	D	494	ILE	5.0
1	C	480	LYS	4.9
1	C	465	ALA	4.9
1	B	523	MET	4.8
1	D	490	ARG	4.8
1	A	471	VAL	4.7
1	A	446	GLU	4.7
1	A	480	LYS	4.7
1	D	463	SER	4.6
1	B	484	LEU	4.5
1	A	477	PRO	4.4
1	C	469	GLN	4.4
1	A	447	GLU	4.3
1	C	471	VAL	4.1
1	D	464	ASP	4.1
1	B	613	GLU	4.1
1	D	694	ALA	4.1
1	A	445	ASN	4.1
1	A	860	GLY	4.1
1	A	746	ILE	4.1
1	B	746	ILE	4.1
1	B	470	LEU	4.0
1	B	481	LEU	4.0
1	C	828	LYS	4.0
1	B	471	VAL	4.0
1	B	469	GLN	4.0
1	A	483	THR	4.0
1	C	468	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	786	PRO	3.8
1	D	693	PRO	3.8
1	B	694	ALA	3.7
1	A	772	VAL	3.7
1	D	772	VAL	3.7
1	A	497	GLN	3.7
1	A	481	LEU	3.7
1	B	630	ARG	3.6
1	C	757	VAL	3.6
1	C	772	VAL	3.5
1	C	740	SER	3.4
1	A	748	GLY	3.4
1	D	627	ARG	3.3
1	A	628	PHE	3.3
1	C	490	ARG	3.3
1	D	695	ALA	3.3
1	B	501	LYS	3.3
1	C	748	GLY	3.3
1	B	747	GLY	3.2
1	D	524	GLY	3.2
1	C	482	GLU	3.2
1	C	485	ILE	3.2
1	C	630	ARG	3.2
1	C	786	PRO	3.2
1	A	444	PRO	3.1
1	B	771	ASN	3.1
1	A	620	GLU	3.1
1	A	474	LYS	3.1
1	A	829	ASP	3.1
1	D	743	ALA	3.1
1	B	693	PRO	3.1
1	D	482	GLU	3.0
1	C	510	GLN	3.0
1	C	524	GLY	3.0
1	B	754	ALA	3.0
1	D	775	SER	3.0
1	D	465	ALA	3.0
1	D	757	VAL	3.0
1	D	745	SER	3.0
1	A	469	GLN	2.9
1	C	464	ASP	2.9
1	C	694	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	472	ASN	2.9
1	C	761	TYR	2.9
1	B	757	VAL	2.9
1	D	746	ILE	2.9
1	B	480	LYS	2.8
1	B	695	ALA	2.8
1	A	789	GLU	2.8
1	D	523	MET	2.8
1	B	482	GLU	2.8
1	A	715	LYS	2.8
1	C	693	PRO	2.8
1	C	616	ALA	2.8
1	C	754	ALA	2.8
1	C	746	ILE	2.8
1	B	698	TRP	2.8
1	A	630	ARG	2.8
1	A	462	LEU	2.8
1	B	773	GLY	2.7
1	C	699	ILE	2.7
1	D	748	GLY	2.7
1	B	748	GLY	2.7
1	C	670	LYS	2.7
1	B	608	TRP	2.7
1	C	481	LEU	2.7
1	A	511	TYR	2.7
1	D	696	ILE	2.7
1	C	548	GLU	2.7
1	D	773	GLY	2.7
1	D	777	CYS	2.6
1	A	498	LEU	2.6
1	D	747	GLY	2.6
1	C	518	ASN	2.6
1	B	677	GLU	2.6
1	D	740	SER	2.6
1	B	741	ALA	2.6
1	D	689	THR	2.6
1	D	768	ALA	2.6
1	C	622	PHE	2.6
1	A	745	SER	2.6
1	D	516	ASP	2.6
1	D	753	ALA	2.6
1	C	474	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	787	THR	2.6
1	A	694	ALA	2.5
1	C	773	GLY	2.5
1	A	510	GLN	2.5
1	B	772	VAL	2.5
1	D	785	GLY	2.5
1	B	749	TYR	2.5
1	A	501	LYS	2.5
1	A	777	CYS	2.5
1	D	774	SER	2.5
1	A	629	ALA	2.5
1	A	769	ALA	2.5
1	C	771	ASN	2.4
1	C	615	PHE	2.4
1	A	771	ASN	2.4
1	D	771	ASN	2.4
1	B	688	CYS	2.4
1	C	747	GLY	2.4
1	A	787	THR	2.4
1	C	698	TRP	2.4
1	A	478	ALA	2.4
1	C	741	ALA	2.4
1	C	511	TYR	2.4
1	C	745	SER	2.4
1	D	469	GLN	2.4
1	B	616	ALA	2.3
1	B	769	ALA	2.3
1	C	753	ALA	2.3
1	B	778	ILE	2.3
1	D	741	ALA	2.3
1	A	756	ILE	2.3
1	D	776	ASN	2.3
1	B	745	SER	2.3
1	C	749	TYR	2.3
1	A	699	ILE	2.3
1	B	740	SER	2.3
1	A	689	THR	2.3
1	B	516	ASP	2.3
1	A	828	LYS	2.2
1	B	777	CYS	2.2
1	A	487	THR	2.2
1	B	753	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	749	TYR	2.2
1	A	468	ILE	2.2
1	B	775	SER	2.2
1	B	597	PRO	2.2
1	A	617	VAL	2.2
1	A	443	ARG	2.2
1	A	490	ARG	2.2
1	D	698	TRP	2.2
1	B	674	TYR	2.2
1	D	511	TYR	2.2
1	B	758	THR	2.2
1	A	523	MET	2.2
1	C	466	GLU	2.2
1	A	693	PRO	2.2
1	C	743	ALA	2.2
1	D	497	GLN	2.1
1	D	744	GLY	2.1
1	C	689	THR	2.1
1	A	753	ALA	2.1
1	B	696	ILE	2.1
1	A	744	GLY	2.1
1	A	747	GLY	2.1
1	D	699	ILE	2.1
1	C	556	ALA	2.1
1	C	695	ALA	2.1
1	C	523	MET	2.1
1	A	773	GLY	2.1
1	B	617	VAL	2.1
1	A	467	ILE	2.1
1	B	743	ALA	2.1
1	A	622	PHE	2.0
1	A	624	SER	2.0
1	C	487	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ADP	B	104	27/27	0.35	6.34	99,101,101,101	0
2	ADP	A	103	27/27	0.32	2.94	93,98,100,100	0
2	ADP	D	105	27/27	0.24	1.46	86,94,100,100	0
2	ADP	A	101	27/27	0.29	1.17	93,96,100,100	0
2	ADP	A	102	27/27	0.30	0.99	94,98,100,100	0
3	117	C	4	41/41	0.15	0.47	37,46,52,53	0
3	117	D	3	41/41	0.15	-0.15	34,44,49,49	0
3	117	B	1	41/41	0.12	-0.46	40,47,50,51	0
3	117	A	2	41/41	0.14	-0.63	34,41,45,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.