



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:16 am GMT

PDB ID : 1HWJ
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH CERIVASTATIN
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

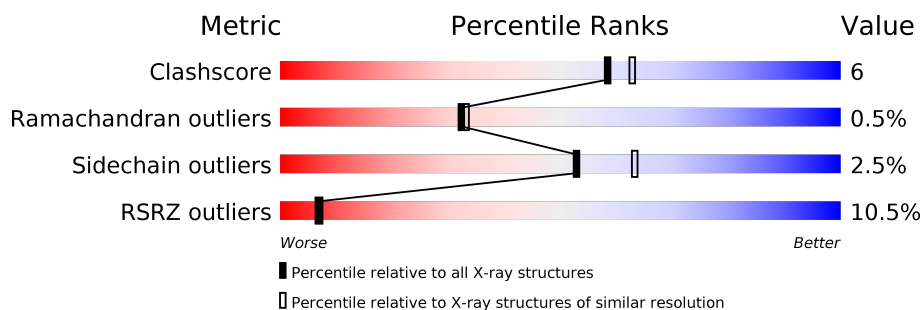
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	467	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	467	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	467	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	467	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	105	-	-	-	X
2	ADP	D	106	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HMG-COA REDUCTASE.

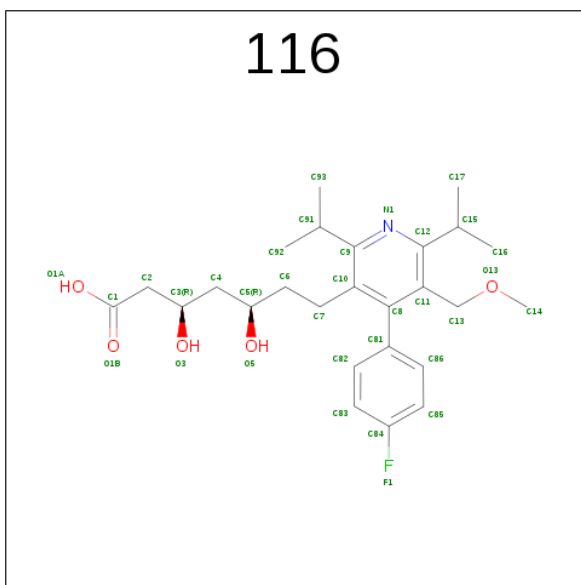
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3052	1900	537	585	30			
1	B	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	C	408	Total	C	N	O	S	0	0	0
			3034	1888	533	583	30			
1	D	392	Total	C	N	O	S	0	0	0
			2900	1803	508	560	29			

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

- # ADP

- Molecule 3 is 7-[4-(4-FLUORO-PHENYL)-5-HYDROXYMETHYL-2,6-DIISOPROPYL-PYRIDIN-3-YL]-3,5-DIHYDROXY-HEPTANOIC ACID (three-letter code: 116) (formula: $C_{26}H_{36}FNO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 33	C 26	F 1	N 1	O 5	0	0
3	A	1	Total 33	C 26	F 1	N 1	O 5	0	0
3	D	1	Total 33	C 26	F 1	N 1	O 5	0	0
3	C	1	Total 33	C 26	F 1	N 1	O 5	0	0

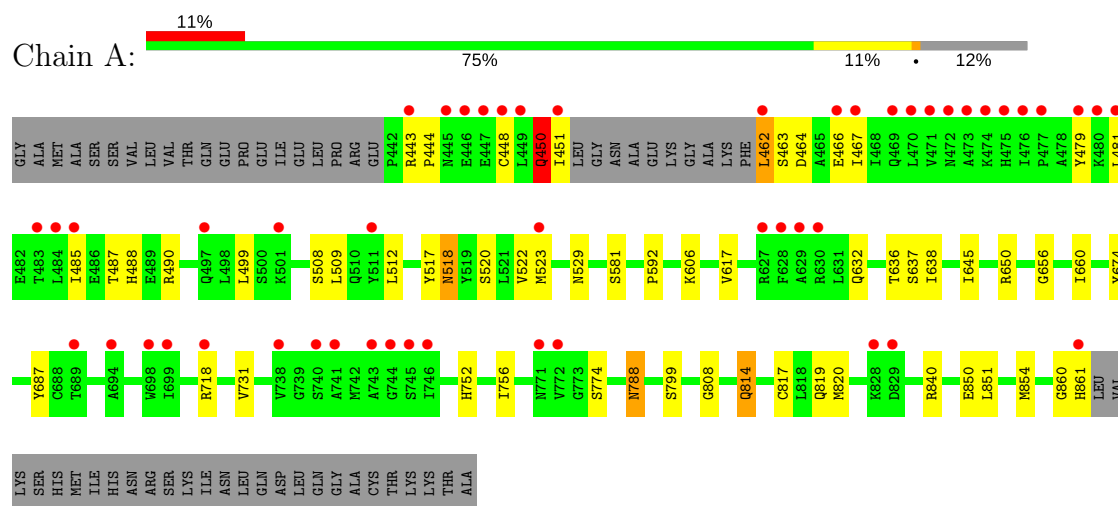
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	52	Total O 52 52	0	0
4	C	33	Total O 33 33	0	0
4	D	49	Total O 49 49	0	0

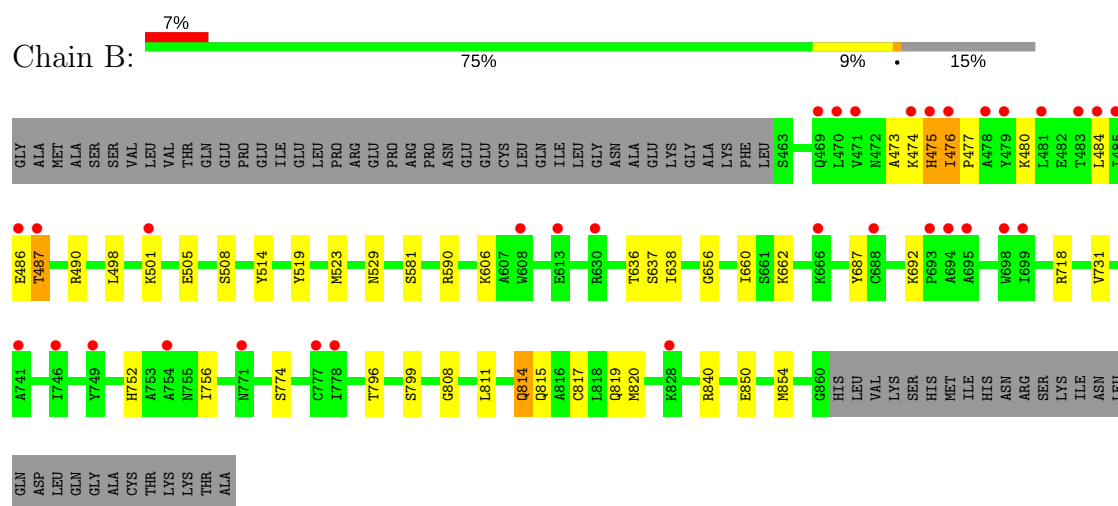
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

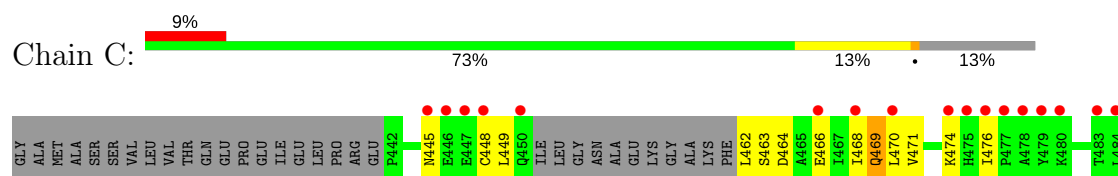
• Molecule 1: HMG-COA REDUCTASE

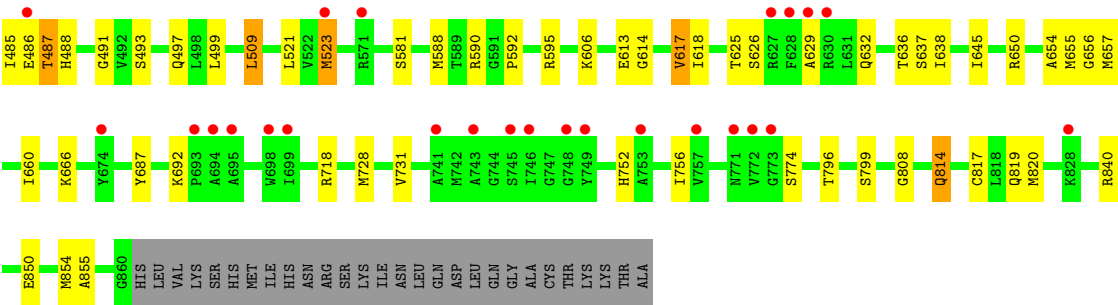


• Molecule 1: HMG-COA REDUCTASE

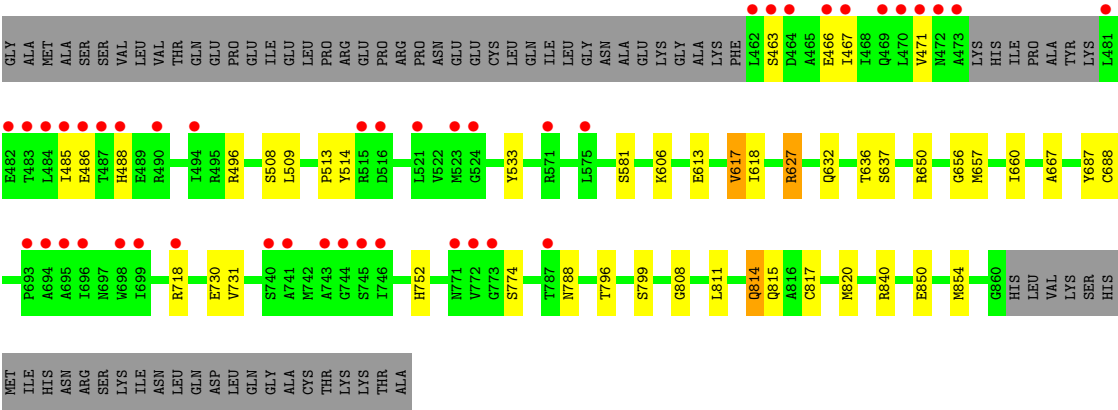


• Molecule 1: HMG-COA REDUCTASE





• Molecule 1: HMG-COA REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.62Å 172.98Å 80.16Å 90.00° 117.35° 90.00°	Depositor
Resolution (Å)	43.50 – 2.26 54.97 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.50-2.26) 93.0 (54.97-2.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.27Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.237 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12418	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 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 116, 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	0/3096	0.66	0/4186
1	B	0.46	0/2994	0.65	0/4049
1	C	0.47	0/3077	0.66	1/4160 (0.0%)
1	D	0.51	0/2938	0.65	0/3972
All	All	0.48	0/12105	0.65	1/16367 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	656	GLY	N-CA-C	5.29	126.34	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3052	0	3087	33	0
1	B	2952	0	2989	29	0
1	C	3034	0	3069	45	0
1	D	2900	0	2934	27	0
2	A	54	0	24	1	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	54	0	24	1	0
2	D	27	0	12	0	0
3	A	33	0	35	2	0
3	B	33	0	35	2	0
3	C	33	0	35	3	0
3	D	33	0	35	1	0
4	A	52	0	0	1	0
4	B	52	0	0	1	0
4	C	33	0	0	1	0
4	D	49	0	0	2	0
All	All	12418	0	12291	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ILE:HG22	1:C:486:GLU:H	1.37	0.89
1:A:487:THR:HG22	1:A:488:HIS:H	1.43	0.83
1:B:523:MET:HE1	4:B:1019:HOH:O	1.81	0.79
1:B:817:CYS:HA	1:B:820:MET:HE3	1.68	0.76
1:D:817:CYS:HA	1:D:820:MET:HE3	1.70	0.74
1:C:817:CYS:HA	1:C:820:MET:HE3	1.70	0.72
3:B:1:116:H91	3:B:1:116:H61	1.73	0.69
1:A:817:CYS:HA	1:A:820:MET:HE3	1.74	0.69
1:C:448:CYS:HB3	1:C:462:LEU:HD22	1.73	0.68
1:A:523:MET:HE1	4:A:1086:HOH:O	1.95	0.67
1:D:688:CYS:SG	4:D:1163:HOH:O	2.54	0.66
1:C:466:GLU:O	1:C:470:LEU:HG	1.96	0.65
1:D:467:ILE:O	1:D:471:VAL:HG23	1.97	0.64
1:C:655:MET:SD	1:C:657:MET:HG2	2.38	0.63
1:C:590:ARG:NH2	1:C:657:MET:HE3	2.14	0.62
1:C:485:ILE:HG22	1:C:486:GLU:N	2.11	0.62
1:C:632:GLN:HE21	1:C:650:ARG:HG3	1.65	0.60
3:A:2:116:H61	3:A:2:116:H91	1.84	0.60
1:D:656:GLY:O	1:D:660:ILE:HG12	2.03	0.58
1:B:476:ILE:HG21	1:B:484:LEU:HD11	1.86	0.57
1:C:588:MET:HB3	1:C:660:ILE:CD1	2.34	0.57
1:D:808:GLY:O	1:D:814:GLN:HG3	2.04	0.57
1:C:581:SER:OG	1:C:840:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:SER:OG	1:D:840:ARG:HD2	2.04	0.57
1:C:523:MET:HE1	4:C:1102:HOH:O	2.03	0.57
1:B:656:GLY:O	1:B:660:ILE:HG12	2.05	0.57
1:B:477:PRO:HD2	1:B:480:LYS:CG	2.35	0.57
1:A:581:SER:OG	1:A:840:ARG:HD2	2.05	0.56
1:C:808:GLY:O	1:C:814:GLN:HG3	2.07	0.55
1:A:656:GLY:O	1:A:660:ILE:HG12	2.06	0.54
1:B:581:SER:OG	1:B:840:ARG:HD2	2.08	0.54
3:C:4:116:H61	3:C:4:116:H91	1.90	0.53
3:D:3:116:H91	3:D:3:116:H61	1.90	0.53
1:C:463:SER:OG	1:C:466:GLU:HG2	2.08	0.53
1:C:654:ALA:HB1	2:C:104:ADP:O1B	2.09	0.52
1:B:519:TYR:O	1:B:523:MET:HG2	2.08	0.52
1:D:627:ARG:HD3	1:D:627:ARG:H	1.75	0.52
1:B:477:PRO:HD2	1:B:480:LYS:HG3	1.92	0.51
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.93	0.51
1:C:625:THR:HG23	1:C:666:LYS:HD3	1.93	0.51
1:A:487:THR:HG22	1:A:488:HIS:N	2.21	0.50
1:B:808:GLY:O	1:B:814:GLN:HG3	2.11	0.50
1:C:632:GLN:NE2	1:C:650:ARG:HG3	2.26	0.50
1:C:626:SER:HB3	1:C:629:ALA:HB2	1.93	0.50
1:D:485:ILE:HG22	1:D:486:GLU:N	2.27	0.50
1:B:774:SER:HA	1:B:799:SER:O	2.13	0.48
1:A:774:SER:HA	1:A:799:SER:O	2.13	0.48
1:D:774:SER:HA	1:D:799:SER:O	2.14	0.48
1:C:606:LYS:HG3	1:C:636:THR:OG1	2.14	0.48
1:C:637:SER:HB2	1:C:687:TYR:OH	2.13	0.48
1:A:448:CYS:HA	1:A:462:LEU:HD21	1.95	0.47
1:A:632:GLN:HE21	1:A:650:ARG:HG3	1.79	0.47
1:A:479:TYR:HB3	1:A:529:ASN:OD1	2.15	0.47
1:C:464:ASP:O	1:C:468:ILE:HG12	2.15	0.47
1:B:637:SER:HB2	1:B:687:TYR:OH	2.15	0.47
1:C:487:THR:OG1	1:C:488:HIS:N	2.48	0.47
1:A:637:SER:HB2	1:A:687:TYR:OH	2.14	0.47
1:C:523:MET:CE	1:C:523:MET:HA	2.45	0.47
1:D:463:SER:HB2	1:D:466:GLU:HG3	1.97	0.47
1:D:637:SER:HB2	1:D:687:TYR:OH	2.15	0.47
1:B:473:ALA:O	1:B:475:HIS:N	2.49	0.46
1:A:518:ASN:ND2	1:A:520:SER:OG	2.49	0.46
1:C:499:LEU:HD23	1:C:509:LEU:HD21	1.98	0.46
1:A:808:GLY:O	1:A:814:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:MET:HB2	1:A:820:MET:HE2	1.73	0.46
1:C:850:GLU:O	1:C:854:MET:HG2	2.14	0.46
1:C:474:LYS:HB2	1:C:476:ILE:HG13	1.98	0.46
1:C:655:MET:CE	1:C:657:MET:HG2	2.45	0.46
1:A:463:SER:HB3	1:A:466:GLU:CD	2.37	0.45
1:C:613:GLU:O	1:C:617:VAL:HG12	2.17	0.45
1:C:774:SER:HA	1:C:799:SER:O	2.16	0.45
1:C:471:VAL:HG13	1:C:476:ILE:O	2.17	0.45
1:A:467:ILE:HD11	1:A:490:ARG:HH21	1.82	0.45
1:A:606:LYS:HG3	1:A:636:THR:OG1	2.17	0.45
1:C:820:MET:HB2	1:C:820:MET:HE2	1.86	0.44
1:B:850:GLU:O	1:B:854:MET:HG2	2.16	0.44
1:A:499:LEU:HD23	1:A:509:LEU:HD21	2.00	0.44
1:D:820:MET:HE2	1:D:820:MET:HB2	1.85	0.44
1:C:485:ILE:HD12	1:C:491:GLY:HA2	1.98	0.44
1:D:850:GLU:O	1:D:854:MET:HG2	2.17	0.44
1:B:638:ILE:O	1:C:796:THR:HG21	2.18	0.44
1:C:592:PRO:HD2	1:C:645:ILE:O	2.17	0.43
1:D:606:LYS:HG3	1:D:636:THR:OG1	2.18	0.43
1:C:614:GLY:O	1:C:618:ILE:HG12	2.17	0.43
1:C:731:VAL:HG12	1:C:854:MET:CE	2.48	0.43
1:A:850:GLU:O	1:A:854:MET:HG2	2.19	0.43
1:B:796:THR:HG21	1:C:638:ILE:O	2.18	0.43
1:A:450:GLN:HB2	1:A:451:ILE:H	1.60	0.43
1:D:731:VAL:HG12	1:D:854:MET:HE3	2.00	0.43
1:B:606:LYS:HG3	1:B:636:THR:OG1	2.18	0.43
1:B:731:VAL:HG12	1:B:854:MET:CE	2.48	0.43
1:C:595:ARG:HH22	1:D:730:GLU:HG2	1.84	0.43
1:A:638:ILE:O	1:D:796:THR:HG21	2.19	0.43
1:A:617:VAL:HG11	1:A:674:TYR:CE1	2.53	0.43
1:A:508:SER:HB2	1:B:819:GLN:CB	2.48	0.42
1:B:498:LEU:O	1:B:501:LYS:HG2	2.20	0.42
2:A:102:ADP:H2	1:B:529:ASN:HD21	1.66	0.42
1:C:692:LYS:HB2	1:C:692:LYS:HE2	1.91	0.42
1:D:618:ILE:HG23	1:D:667:ALA:HB1	2.02	0.42
1:A:731:VAL:HG12	1:A:854:MET:CE	2.49	0.42
1:B:486:GLU:O	1:B:487:THR:HB	2.20	0.42
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.80	0.42
1:A:632:GLN:NE2	1:A:650:ARG:HG3	2.34	0.42
1:D:731:VAL:HG12	1:D:854:MET:CE	2.50	0.42
1:A:481:LEU:O	1:A:485:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ILE:HD12	1:A:756:ILE:N	2.34	0.42
1:A:819:GLN:CB	1:B:508:SER:HB2	2.50	0.42
1:D:627:ARG:N	1:D:627:ARG:HD3	2.35	0.42
1:D:811:LEU:O	1:D:815:GLN:HG3	2.19	0.42
1:C:756:ILE:HD12	1:C:756:ILE:N	2.35	0.41
1:D:513:PRO:HB2	1:D:533:TYR:CZ	2.55	0.41
1:D:613:GLU:O	1:D:617:VAL:HG13	2.20	0.41
1:B:692:LYS:HB2	1:B:692:LYS:HE2	1.94	0.41
1:C:731:VAL:HG12	1:C:854:MET:HE3	2.01	0.41
1:A:462:LEU:HB2	1:A:463:SER:H	1.52	0.41
1:A:788:ASN:HA	1:A:788:ASN:HD22	1.68	0.41
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.80	0.41
3:A:2:116:C86	3:A:2:116:H72	2.51	0.41
1:A:592:PRO:HD2	1:A:645:ILE:O	2.20	0.41
1:A:517:TYR:HE2	1:A:522:VAL:HG21	1.86	0.41
1:B:662:LYS:HB3	1:B:662:LYS:HE2	1.93	0.41
1:B:476:ILE:HG22	1:B:480:LYS:HB2	2.02	0.41
3:C:4:116:C86	3:C:4:116:H72	2.51	0.41
1:C:493:SER:O	1:C:497:GLN:HG3	2.21	0.41
1:D:496:ARG:NH2	1:D:509:LEU:O	2.53	0.41
1:B:811:LEU:O	1:B:815:GLN:HG3	2.21	0.41
3:B:1:116:C91	3:B:1:116:H61	2.46	0.40
3:C:4:116:C91	3:C:4:116:H61	2.51	0.40
1:C:728:MET:SD	1:C:855:ALA:HA	2.61	0.40
1:A:443:ARG:HA	1:A:444:PRO:HD3	1.86	0.40
1:B:756:ILE:HD12	1:B:756:ILE:N	2.36	0.40
1:C:445:ASN:OD1	1:C:469:GLN:HB3	2.21	0.40
1:C:819:GLN:HB2	1:D:508:SER:HB2	2.02	0.40
1:D:632:GLN:HE21	1:D:650:ARG:HG3	1.85	0.40
1:D:657:MET:HG2	4:D:1186:HOH: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	406/467 (87%)	386 (95%)	18 (4%)	2 (0%)	32	33
1	B	396/467 (85%)	375 (95%)	17 (4%)	4 (1%)	18	15
1	C	404/467 (86%)	379 (94%)	24 (6%)	1 (0%)	51	60
1	D	388/467 (83%)	371 (96%)	16 (4%)	1 (0%)	44	50
All	All	1594/1868 (85%)	1511 (95%)	75 (5%)	8 (0%)	32	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	860	GLY
1	B	474	LYS
1	B	475	HIS
1	B	487	THR
1	C	449	LEU
1	B	514	TYR
1	D	514	TYR

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	328/375 (88%)	317 (97%)	11 (3%)	42	52
1	B	316/375 (84%)	311 (98%)	5 (2%)	68	78
1	C	326/375 (87%)	317 (97%)	9 (3%)	49	58
1	D	311/375 (83%)	304 (98%)	7 (2%)	56	65
All	All	1281/1500 (85%)	1249 (98%)	32 (2%)	53	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	462	LEU
1	A	464	ASP
1	A	512	LEU
1	A	518	ASN
1	A	718	ARG
1	A	752	HIS
1	A	788	ASN
1	A	814	GLN
1	A	851	LEU
1	A	861	HIS
1	B	476	ILE
1	B	505	GLU
1	B	718	ARG
1	B	752	HIS
1	B	814	GLN
1	C	469	GLN
1	C	487	THR
1	C	509	LEU
1	C	521	LEU
1	C	523	MET
1	C	617	VAL
1	C	718	ARG
1	C	752	HIS
1	C	814	GLN
1	D	488	HIS
1	D	617	VAL
1	D	627	ARG
1	D	718	ARG
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	635	HIS
1	A	788	ASN
1	A	819	GLN
1	B	469	GLN
1	B	488	HIS
1	B	635	HIS

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Mol	Chain	Res	Type
1	B	819	GLN
1	C	450	GLN
1	C	469	GLN
1	C	510	GLN
1	C	632	GLN
1	C	635	HIS
1	C	819	GLN
1	D	469	GLN
1	D	635	HIS
1	D	788	ASN
1	D	819	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	-	25,29,29	1.15	1 (4%)	24,45,45	0.87	0
2	ADP	A	102	-	25,29,29	1.24	2 (8%)	24,45,45	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	116	A	2	-	31,34,34	2.03	6 (19%)	34,47,47	1.42	3 (8%)
3	116	B	1	-	31,34,34	2.12	8 (25%)	34,47,47	1.49	4 (11%)
2	ADP	B	105	-	25,29,29	1.54	6 (24%)	24,45,45	0.82	0
2	ADP	C	103	-	25,29,29	1.26	2 (8%)	24,45,45	1.09	1 (4%)
2	ADP	C	104	-	25,29,29	1.31	3 (12%)	24,45,45	0.75	0
3	116	C	4	-	31,34,34	2.11	6 (19%)	34,47,47	1.51	3 (8%)
2	ADP	D	106	-	25,29,29	1.39	4 (16%)	24,45,45	0.77	0
3	116	D	3	-	31,34,34	2.21	7 (22%)	34,47,47	1.33	2 (5%)

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	-	-	0/12/32/32	0/3/3/3
2	ADP	A	102	-	-	0/12/32/32	0/3/3/3
3	116	A	2	-	-	0/26/28/28	0/2/2/2
3	116	B	1	-	-	0/26/28/28	0/2/2/2
2	ADP	B	105	-	-	0/12/32/32	0/3/3/3
2	ADP	C	103	-	-	0/12/32/32	0/3/3/3
2	ADP	C	104	-	-	0/12/32/32	0/3/3/3
3	116	C	4	-	-	0/26/28/28	0/2/2/2
2	ADP	D	106	-	-	0/12/32/32	0/3/3/3
3	116	D	3	-	-	0/26/28/28	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	116	C8-C81	-6.38	1.38	1.50
3	C	4	116	C8-C81	-5.55	1.40	1.50
3	B	1	116	C8-C81	-5.30	1.40	1.50
3	A	2	116	C8-C81	-5.05	1.40	1.50
3	D	3	116	C6-C7	-4.25	1.33	1.53
3	A	2	116	C6-C7	-4.04	1.34	1.53
3	C	4	116	C6-C7	-4.03	1.34	1.53
3	B	1	116	C6-C7	-3.71	1.35	1.53
2	C	103	ADP	C8-N7	-3.61	1.27	1.34
2	D	106	ADP	C8-N7	-3.31	1.28	1.34
2	A	101	ADP	C8-N7	-3.23	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	ADP	C8-N7	-3.20	1.28	1.34
2	B	105	ADP	C8-N7	-3.14	1.28	1.34
2	C	104	ADP	C8-N7	-3.09	1.28	1.34
3	D	3	116	C9-N1	-2.06	1.31	1.34
2	B	105	ADP	C5-C4	-2.04	1.35	1.40
3	D	3	116	C13-C11	2.09	1.55	1.51
2	C	103	ADP	C2'-C3'	2.09	1.59	1.53
3	C	4	116	C83-C84	2.15	1.41	1.37
2	B	105	ADP	O2'-C2'	2.17	1.47	1.43
2	D	106	ADP	C2'-C3'	2.20	1.59	1.53
2	A	102	ADP	O4'-C4'	2.22	1.50	1.45
3	D	3	116	C8-C11	2.22	1.45	1.40
3	B	1	116	C8-C10	2.22	1.45	1.40
2	C	104	ADP	O4'-C1'	2.29	1.44	1.41
3	A	2	116	C7-C10	2.36	1.56	1.52
3	A	2	116	C4-C5	2.40	1.57	1.52
2	D	106	ADP	O4'-C1'	2.43	1.44	1.41
3	B	1	116	C7-C10	2.43	1.56	1.52
2	B	105	ADP	C2'-C3'	2.50	1.60	1.53
3	B	1	116	C8-C11	2.51	1.45	1.40
2	D	106	ADP	O4'-C4'	2.66	1.51	1.45
2	C	104	ADP	O4'-C4'	2.69	1.51	1.45
3	C	4	116	C7-C10	2.96	1.57	1.52
2	B	105	ADP	O4'-C4'	2.98	1.51	1.45
3	B	1	116	C13-C11	3.19	1.57	1.51
2	B	105	ADP	O4'-C1'	3.43	1.46	1.41
3	A	2	116	C9-C91	3.94	1.56	1.51
3	D	3	116	C9-C91	4.38	1.56	1.51
3	B	1	116	C9-C91	4.50	1.57	1.51
3	C	4	116	C9-C91	4.53	1.57	1.51
3	B	1	116	C12-C15	5.21	1.58	1.51
3	C	4	116	C12-C15	5.42	1.58	1.51
3	A	2	116	C12-C15	5.45	1.58	1.51
3	D	3	116	C12-C15	6.50	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	116	C85-C84-C83	-2.01	120.06	122.86
3	A	2	116	O13-C13-C11	2.01	111.95	108.46
3	C	4	116	C92-C91-C9	2.16	114.99	111.21
3	B	1	116	O13-C13-C11	2.37	112.58	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	103	ADP	C4'-O4'-C1'	2.78	112.73	109.77
3	D	3	116	C6-C7-C10	3.60	122.16	112.11
3	C	4	116	C6-C7-C10	3.83	122.78	112.11
3	A	2	116	C6-C7-C10	4.17	123.73	112.11
3	B	1	116	C6-C7-C10	4.31	124.12	112.11
3	A	2	116	C7-C6-C5	5.10	125.06	115.31
3	B	1	116	C7-C6-C5	5.15	125.14	115.31
3	D	3	116	C7-C6-C5	5.31	125.44	115.31
3	C	4	116	C7-C6-C5	5.95	126.68	115.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	ADP	1	0
3	A	2	116	2	0
3	B	1	116	2	0
2	C	104	ADP	1	0
3	C	4	116	3	0
3	D	3	116	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	410/467 (87%)	0.51	50 (12%) 5 4	27, 51, 99, 101	0
1	B	398/467 (85%)	0.49	33 (8%) 12 13	30, 50, 86, 101	0
1	C	408/467 (87%)	0.64	42 (10%) 7 7	30, 53, 100, 101	0
1	D	392/467 (83%)	0.47	44 (11%) 6 5	29, 48, 93, 101	0
All	All	1608/1868 (86%)	0.53	169 (10%) 7 7	27, 50, 99, 101	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	475	HIS	7.8
1	D	483	THR	7.6
1	B	471	VAL	7.5
1	D	462	LEU	7.3
1	A	861	HIS	7.1
1	A	484	LEU	6.8
1	A	473	ALA	6.7
1	D	484	LEU	6.6
1	C	483	THR	6.4
1	B	475	HIS	6.3
1	D	486	GLU	6.1
1	D	469	GLN	6.1
1	A	449	LEU	5.9
1	D	471	VAL	5.8
1	D	523	MET	5.7
1	A	475	HIS	5.6
1	C	484	LEU	5.3
1	D	470	LEU	5.3
1	A	448	CYS	5.2
1	B	476	ILE	5.2
1	C	486	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	4.9
1	C	477	PRO	4.7
1	D	485	ILE	4.6
1	D	524	GLY	4.5
1	B	470	LEU	4.5
1	A	451	ILE	4.4
1	B	486	GLU	4.3
1	B	485	ILE	4.3
1	B	613	GLU	4.2
1	A	471	VAL	4.2
1	A	470	LEU	4.2
1	D	467	ILE	4.2
1	D	487	THR	4.1
1	A	479	TYR	4.1
1	D	481	LEU	4.0
1	D	694	ALA	4.0
1	A	446	GLU	3.9
1	B	487	THR	3.9
1	C	448	CYS	3.9
1	C	447	GLU	3.8
1	D	473	ALA	3.8
1	A	828	LYS	3.7
1	A	467	ILE	3.6
1	B	479	TYR	3.5
1	C	627	ARG	3.5
1	A	630	ARG	3.4
1	C	476	ILE	3.4
1	C	628	PHE	3.4
1	D	693	PRO	3.4
1	A	472	ASN	3.4
1	D	695	ALA	3.3
1	B	746	ILE	3.3
1	D	494	ILE	3.3
1	D	482	GLU	3.3
1	B	698	TRP	3.2
1	C	450	GLN	3.2
1	C	828	LYS	3.2
1	D	466	GLU	3.2
1	C	699	ILE	3.1
1	A	718	ARG	3.1
1	A	469	GLN	3.1
1	A	477	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	743	ALA	3.1
1	B	630	ARG	3.1
1	B	694	ALA	3.1
1	C	695	ALA	3.1
1	B	608	TRP	3.0
1	D	718	ARG	3.0
1	C	746	ILE	3.0
1	D	472	ASN	3.0
1	C	446	GLU	3.0
1	D	463	SER	3.0
1	C	445	ASN	3.0
1	A	741	ALA	3.0
1	A	699	ILE	2.9
1	A	481	LEU	2.9
1	A	447	GLU	2.9
1	C	630	ARG	2.9
1	C	479	TYR	2.9
1	C	749	TYR	2.9
1	A	462	LEU	2.9
1	A	627	ARG	2.9
1	B	474	LYS	2.9
1	B	484	LEU	2.9
1	C	694	ALA	2.9
1	C	693	PRO	2.8
1	A	698	TRP	2.8
1	C	698	TRP	2.8
1	D	772	VAL	2.8
1	A	497	GLN	2.7
1	D	746	ILE	2.7
1	C	523	MET	2.7
1	D	516	ASP	2.7
1	D	699	ILE	2.7
1	B	688	CYS	2.7
1	D	698	TRP	2.7
1	B	699	ILE	2.7
1	A	466	GLU	2.6
1	B	666	LYS	2.6
1	B	483	THR	2.6
1	C	480	LYS	2.6
1	A	474	LYS	2.6
1	C	745	SER	2.6
1	B	695	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	771	ASN	2.6
1	C	757	VAL	2.5
1	D	490	ARG	2.5
1	C	629	ALA	2.5
1	C	674	TYR	2.5
1	D	488	HIS	2.5
1	B	828	LYS	2.5
1	C	470	LEU	2.5
1	A	485	ILE	2.5
1	B	478	ALA	2.4
1	B	741	ALA	2.4
1	D	773	GLY	2.4
1	B	693	PRO	2.4
1	C	773	GLY	2.4
1	D	464	ASP	2.3
1	B	481	LEU	2.3
1	D	575	LEU	2.3
1	D	745	SER	2.3
1	B	754	ALA	2.3
1	C	753	ALA	2.3
1	A	445	ASN	2.3
1	C	466	GLU	2.3
1	A	746	ILE	2.3
1	A	689	THR	2.3
1	B	469	GLN	2.3
1	A	744	GLY	2.3
1	C	571	ARG	2.3
1	A	772	VAL	2.3
1	D	696	ILE	2.3
1	A	743	ALA	2.2
1	C	741	ALA	2.2
1	C	772	VAL	2.2
1	A	628	PHE	2.2
1	A	483	THR	2.2
1	C	468	ILE	2.2
1	A	829	ASP	2.2
1	A	771	ASN	2.2
1	C	743	ALA	2.2
1	C	474	LYS	2.2
1	D	521	LEU	2.2
1	A	501	LYS	2.2
1	A	523	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	745	SER	2.1
1	B	501	LYS	2.1
1	D	515	ARG	2.1
1	D	571	ARG	2.1
1	C	478	ALA	2.1
1	D	741	ALA	2.1
1	B	778	ILE	2.1
1	B	771	ASN	2.1
1	A	443	ARG	2.1
1	D	744	GLY	2.1
1	A	629	ALA	2.1
1	D	771	ASN	2.1
1	A	511	TYR	2.1
1	B	749	TYR	2.1
1	D	740	SER	2.1
1	D	787	THR	2.1
1	A	694	ALA	2.1
1	A	740	SER	2.0
1	A	738	VAL	2.0
1	B	777	CYS	2.0
1	A	480	LYS	2.0
1	C	748	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	B	105	27/27	0.54	0.32	5.62	99,100,100,100	0
2	ADP	D	106	27/27	0.72	0.30	4.12	99,100,100,100	0
2	ADP	C	103	27/27	0.68	0.32	1.54	91,95,100,100	0
2	ADP	C	104	27/27	0.82	0.25	1.18	98,100,100,100	0
2	ADP	A	102	27/27	0.79	0.24	0.72	86,91,100,100	0
3	116	C	4	33/33	0.93	0.16	0.44	39,45,48,50	0
3	116	B	1	33/33	0.93	0.16	0.44	42,49,54,55	0
2	ADP	A	101	27/27	0.81	0.22	0.32	88,92,100,100	0
3	116	D	3	33/33	0.96	0.15	0.08	39,46,49,49	0
3	116	A	2	33/33	0.96	0.15	-0.09	35,40,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.