



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:47 PM GMT

PDB ID : 1HW9
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH SIMVASTATIN
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.33 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>

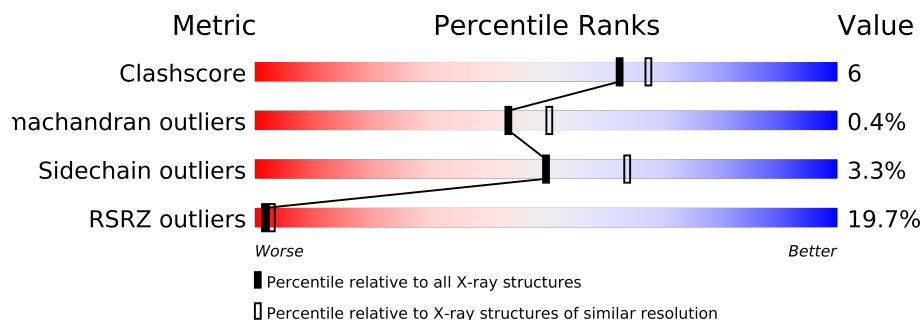
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.33 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	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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	

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	B	104	-	X
2	ADP	D	105	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12185 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
			3037	1892	533	582	30			
1	B	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	C	389	Total	C	N	O	S	0	0	0
			2881	1792	504	556	29			
1	D	388	Total	C	N	O	S	0	0	0
			2880	1792	504	555	29			

There are 20 discrepancies between the modelled and reference sequences:

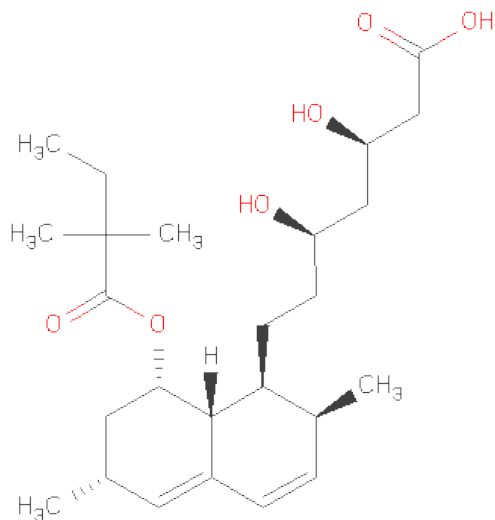
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	INSERTION	UNP P04035
A	423	ALA	-	INSERTION	UNP P04035
A	424	MET	-	INSERTION	UNP P04035
A	425	ALA	-	INSERTION	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	422	GLY	-	INSERTION	UNP P04035
B	423	ALA	-	INSERTION	UNP P04035
B	424	MET	-	INSERTION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

- Molecule 3 is SIMVASTATIN ACID (three-letter code: SIM) (formula: $C_{25}H_{40}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			31	25	6		
3	C	1	Total	C	O	0	0
			31	25	6		
3	B	1	Total	C	O	0	0
			31	25	6		
3	A	1	Total	C	O	0	0
			31	25	6		

- Molecule 4 is water.

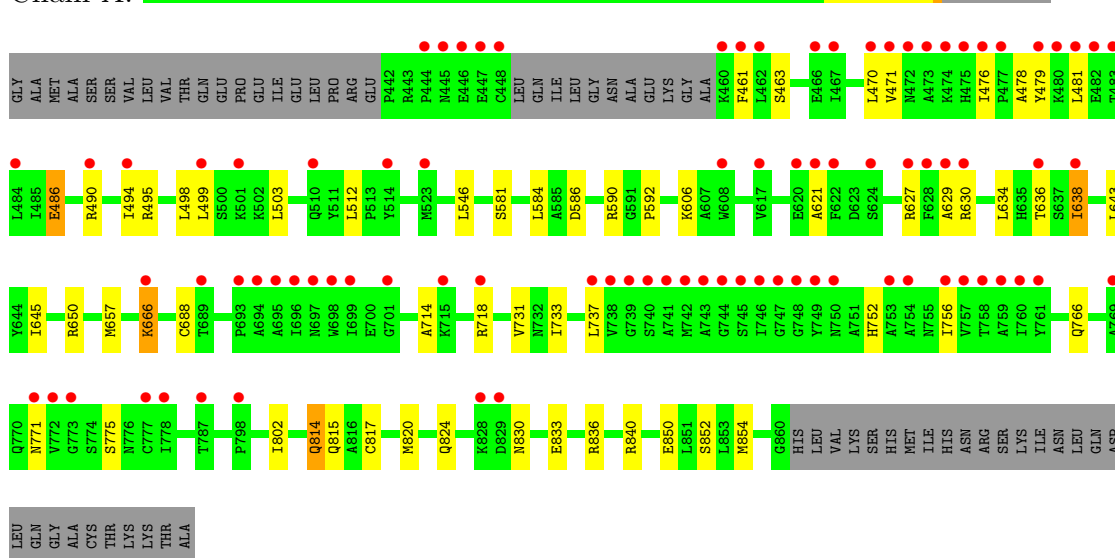
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	49	Total	O	0	0
			49	49		
4	C	33	Total	O	0	0
			33	33		
4	D	50	Total	O	0	0
			50	50		

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.

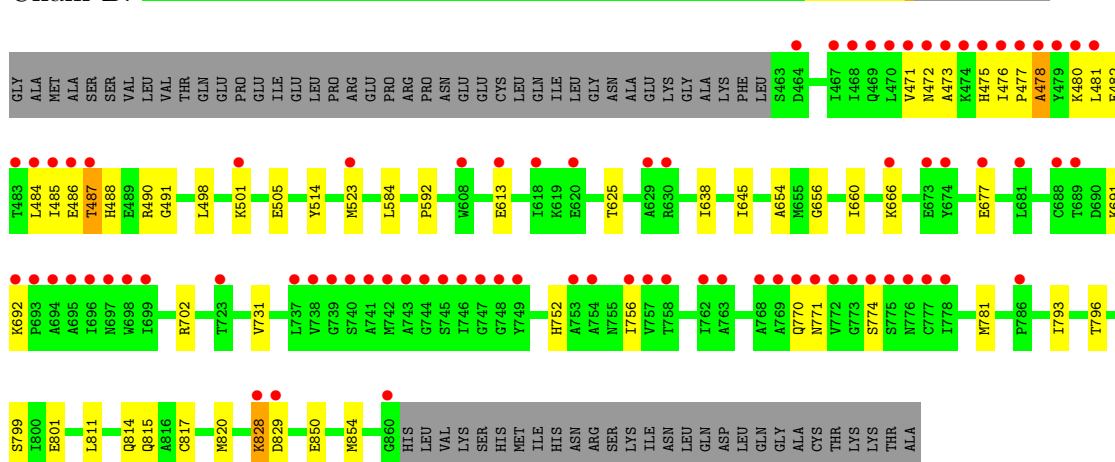
• Molecule 1: HMG-COA REDUCTASE

Chain A:



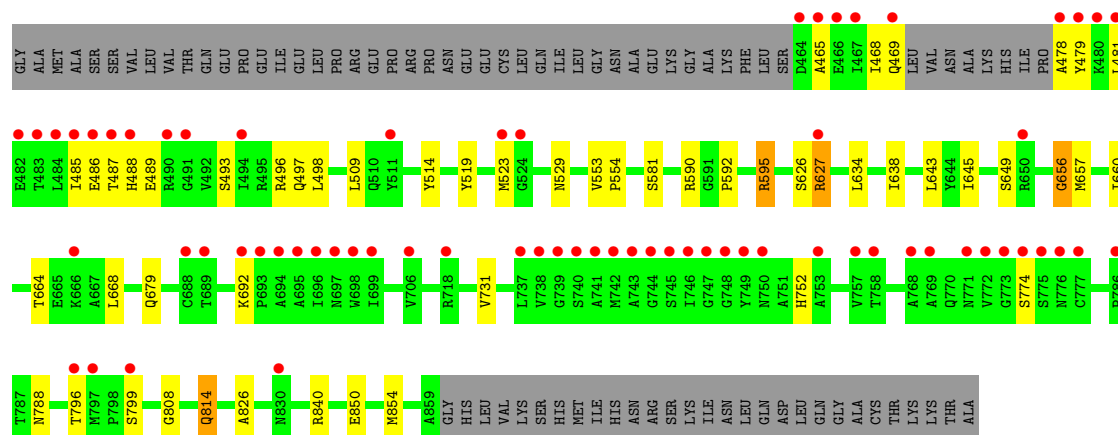
• Molecule 1: HMG-COA REDUCTASE

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	74.55Å 172.82Å 80.03Å 90.00° 117.56° 90.00°	Depositor
Resolution (Å)	43.43 – 2.33 52.40 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.43-2.33) 91.8 (52.40-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.32Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.248 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
Estimated twinning fraction	0.019 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 73786 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: SIM, 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	0.44	0/3081	0.63	0/4164
1	B	0.43	0/2994	0.63	0/4049
1	C	0.41	0/2920	0.62	0/3946
1	D	0.46	0/2919	0.63	1/3945 (0.0%)
All	All	0.44	0/11914	0.63	1/16104 (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	D	656	GLY	N-CA-C	5.09	125.82	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	3037	0	3072	37	0
1	B	2952	0	2989	39	0
1	C	2881	0	2911	31	0
1	D	2880	0	2911	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	12	0	0
2	B	54	0	24	1	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
3	A	31	0	39	0	0
3	B	31	0	39	0	0
3	C	62	0	78	1	0
4	A	44	0	0	0	0
4	B	49	0	0	0	0
4	C	33	0	0	0	0
4	D	50	0	0	0	0
All	All	12185	0	12099	136	0

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

All (136) 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	1.46	0.98
1:C:485:ILE:HG22	1:C:486:GLU:H	1.45	0.82
1:B:817:CYS:HA	1:B:820:MET:HE3	1.69	0.75
1:A:479:TYR:HA	1:A:495:ARG:HH21	1.54	0.72
1:D:808:GLY:O	1:D:814:GLN:HG3	1.93	0.69
1:D:488:HIS:HD2	1:D:523:MET:HG3	1.58	0.68
1:B:654:ALA:HB1	2:B:104:ADP:O1B	1.93	0.68
1:A:584:LEU:HD11	1:D:638:ILE:HD11	1.75	0.67
1:B:485:ILE:HG22	1:B:486:GLU:H	1.60	0.67
1:A:714:ALA:HB1	1:A:718:ARG:NH1	2.09	0.66
1:D:519:TYR:O	1:D:523:MET:HG2	1.96	0.66
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.78	0.66
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.78	0.65
1:A:629:ALA:O	1:A:630:ARG:HD2	1.96	0.64
1:D:656:GLY:O	1:D:660:ILE:HG12	1.97	0.64
1:B:485:ILE:HG22	1:B:486:GLU:N	2.13	0.64
1:B:656:GLY:O	1:B:660:ILE:HG12	1.99	0.63
1:B:781:MET:HE2	1:B:793:ILE:HD12	1.82	0.62
1:D:638:ILE:HG22	1:D:643:LEU:HD13	1.81	0.62
1:C:808:GLY:O	1:C:814:GLN:HG3	2.00	0.61
1:B:850:GLU:O	1:B:854:MET:HG2	2.01	0.60
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.02	0.59
1:A:731:VAL:HG12	1:A:854:MET:CE	2.32	0.59
1:A:714:ALA:HB1	1:A:718:ARG:HH12	1.67	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:485:ILE:HD11	1:C:494:ILE:HD12	1.85	0.58
1:C:850:GLU:O	1:C:854:MET:HG2	2.03	0.58
1:D:486:GLU:HG2	1:D:487:THR:H	1.67	0.58
1:A:606:LYS:HG3	1:A:636:THR:HG21	1.85	0.58
1:D:486:GLU:HG2	1:D:487:THR:N	2.20	0.57
1:B:584:LEU:HD22	1:C:638:ILE:HD12	1.86	0.57
1:D:581:SER:OG	1:D:840:ARG:HD2	2.05	0.57
1:C:480:LYS:O	1:C:484:LEU:HG	2.04	0.57
1:A:586:ASP:HB3	1:A:650:ARG:HE	1.70	0.56
1:C:581:SER:OG	1:C:840:ARG:HD2	2.05	0.56
1:D:850:GLU:O	1:D:854:MET:HG2	2.04	0.56
1:B:482:GLU:HG2	1:B:523:MET:HG2	1.88	0.56
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.88	0.55
1:A:756:ILE:HD12	1:A:756:ILE:N	2.21	0.55
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.89	0.55
1:C:482:GLU:HG2	1:C:523:MET:HG2	1.87	0.55
1:D:649:SER:HB3	1:D:660:ILE:HD12	1.89	0.55
1:D:485:ILE:HG22	1:D:486:GLU:N	2.23	0.55
1:A:581:SER:OG	1:A:840:ARG:HD2	2.07	0.54
1:A:731:VAL:HG12	1:A:854:MET:HE1	1.90	0.54
1:B:477:PRO:HG2	1:B:480:LYS:HZ3	1.73	0.54
1:A:817:CYS:HA	1:A:820:MET:HE3	1.89	0.53
1:D:493:SER:O	1:D:497:GLN:HG3	2.08	0.53
1:A:606:LYS:HG3	1:A:636:THR:CG2	2.39	0.53
1:C:656:GLY:O	1:C:660:ILE:HG12	2.09	0.52
1:B:475:HIS:O	1:B:476:ILE:HG13	2.10	0.52
1:B:828:LYS:CD	1:B:829:ASP:H	2.23	0.51
1:A:621:ALA:HB1	1:A:666:LYS:HE3	1.93	0.50
1:B:691:LYS:HE2	1:B:770:GLN:HG3	1.93	0.50
1:B:811:LEU:O	1:B:815:GLN:HG3	2.12	0.50
1:B:471:VAL:C	1:B:473:ALA:H	2.15	0.50
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.41	0.50
1:A:627:ARG:H	1:A:627:ARG:HD3	1.76	0.49
1:B:477:PRO:HG2	1:B:480:LYS:NZ	2.27	0.49
1:B:731:VAL:HG12	1:B:854:MET:CE	2.43	0.49
1:C:768:ALA:O	1:C:771:ASN:HB3	2.13	0.49
1:D:731:VAL:HG12	1:D:854:MET:HE3	1.95	0.48
1:C:731:VAL:HG12	1:C:854:MET:CE	2.43	0.48
1:C:479:TYR:HB3	1:C:529:ASN:OD1	2.13	0.48
1:A:592:PRO:HD2	1:A:645:ILE:O	2.13	0.48
1:C:485:ILE:HG22	1:C:486:GLU:N	2.23	0.48
1:D:468:ILE:HG23	1:D:498:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:826:ALA:HB1	2:D:105:ADP:HN61	1.79	0.47
1:B:731:VAL:HG12	1:B:854:MET:HE3	1.96	0.47
1:C:731:VAL:HG12	1:C:854:MET:HE3	1.96	0.47
1:A:850:GLU:O	1:A:854:MET:HG2	2.15	0.47
1:B:477:PRO:O	1:B:478:ALA:CB	2.62	0.47
1:C:632:GLN:HE21	1:C:650:ARG:HG2	1.80	0.47
1:D:496:ARG:NH2	1:D:509:LEU:O	2.48	0.47
1:A:638:ILE:O	1:D:796:THR:HG21	2.15	0.47
1:B:592:PRO:HD2	1:B:645:ILE:O	2.14	0.47
1:A:771:ASN:ND2	1:A:775:SER:OG	2.48	0.47
1:C:463:SER:O	1:C:467:ILE:HG12	2.15	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.15	0.46
1:D:731:VAL:HG12	1:D:854:MET:CE	2.45	0.46
1:D:487:THR:HG22	1:D:489:GLU:H	1.80	0.46
1:B:702:ARG:HD3	1:B:801:GLU:OE2	2.15	0.46
1:B:828:LYS:HD3	1:B:829:ASP:H	1.81	0.46
1:B:482:GLU:HG3	1:B:488:HIS:HD2	1.81	0.46
1:D:479:TYR:HB3	1:D:529:ASN:OD1	2.16	0.45
1:B:476:ILE:HD13	1:B:484:LEU:CD2	2.46	0.45
1:D:488:HIS:CD2	1:D:523:MET:HG3	2.46	0.45
1:B:498:LEU:O	1:B:501:LYS:HG2	2.17	0.45
1:B:828:LYS:HD3	1:B:829:ASP:N	2.31	0.45
1:D:626:SER:HA	1:D:627:ARG:HH11	1.82	0.45
1:C:518:ASN:ND2	1:C:520:SER:OG	2.50	0.44
1:D:592:PRO:HD2	1:D:645:ILE:O	2.18	0.44
1:C:592:PRO:HD2	1:C:645:ILE:O	2.16	0.44
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.84	0.44
1:C:480:LYS:NZ	1:C:480:LYS:HB3	2.33	0.44
1:A:815:GLN:HG2	1:A:824:GLN:CG	2.48	0.44
1:B:638:ILE:O	1:C:796:THR:HG21	2.18	0.44
1:B:477:PRO:HD2	1:B:480:LYS:HD2	2.00	0.43
1:C:614:GLY:O	1:C:617:VAL:HG13	2.18	0.43
1:A:471:VAL:HG13	1:A:476:ILE:O	2.17	0.43
1:C:478:ALA:O	1:C:481:LEU:HG	2.18	0.43
1:A:731:VAL:HG12	1:A:854:MET:HE3	2.00	0.43
1:A:650:ARG:HH11	1:A:650:ARG:HG3	1.84	0.43
1:D:485:ILE:HG22	1:D:486:GLU:H	1.83	0.43
1:D:478:ALA:O	1:D:481:LEU:HG	2.18	0.43
1:A:490:ARG:O	1:A:494:ILE:HG12	2.19	0.43
1:C:553:VAL:HA	1:C:554:PRO:HD2	1.93	0.43
1:C:690:ASP:OD2	3:C:1:SIM:H41	2.18	0.42
1:A:546:LEU:HD11	1:A:581:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:733:ILE:O	1:A:737:LEU:HB2	2.19	0.42
1:D:627:ARG:NH1	1:D:627:ARG:H	2.18	0.42
1:B:485:ILE:CG2	1:B:486:GLU:N	2.82	0.42
1:A:830:ASN:O	1:A:833:GLU:HB2	2.19	0.42
1:D:774:SER:HA	1:D:799:SER:O	2.20	0.42
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.85	0.42
1:A:836:ARG:O	1:A:840:ARG:HG3	2.20	0.42
1:C:788:ASN:HA	1:C:788:ASN:HD22	1.65	0.42
1:A:657:MET:CE	1:A:657:MET:HA	2.50	0.42
1:C:649:SER:HB3	1:C:660:ILE:HD12	2.00	0.42
1:A:629:ALA:C	1:A:630:ARG:HD2	2.40	0.41
1:B:692:LYS:HB2	1:B:692:LYS:HE2	1.89	0.41
1:B:475:HIS:C	1:B:476:ILE:HG13	2.41	0.41
1:D:664:THR:O	1:D:668:LEU:HG	2.21	0.41
1:D:692:LYS:HB2	1:D:692:LYS:HE2	1.91	0.41
1:D:826:ALA:HB1	2:D:105:ADP:N6	2.35	0.41
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.84	0.41
1:A:814:GLN:H	1:A:814:GLN:NE2	2.19	0.41
1:D:553:VAL:HA	1:D:554:PRO:HD2	1.95	0.40
1:A:478:ALA:O	1:A:481:LEU:HG	2.21	0.40
1:C:613:GLU:O	1:C:617:VAL:HG12	2.21	0.40
1:C:637:SER:HB2	1:C:687:TYR:OH	2.21	0.40
1:C:774:SER:HA	1:C:799:SER:O	2.21	0.40
1:B:478:ALA:O	1:B:481:LEU:HG	2.22	0.40
1:B:487:THR:HG23	1:B:490:ARG:CB	2.50	0.40
1:B:774:SER:HA	1:B:799:SER:O	2.22	0.40
1:D:595:ARG:HD2	1:D:679:GLN:OE1	2.21	0.40
1:B:756:ILE:HD12	1:B:756:ILE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	404/467 (86%)	381 (94%)	22 (5%)	1 (0%)	56 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	396/467 (85%)	373 (94%)	20 (5%)	3 (1%)	27	30
1	C	385/467 (82%)	364 (94%)	20 (5%)	1 (0%)	50	60
1	D	384/467 (82%)	365 (95%)	17 (4%)	2 (0%)	38	44
All	All	1569/1868 (84%)	1483 (94%)	79 (5%)	7 (0%)	43	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLU
1	D	465	ALA
1	B	478	ALA
1	B	514	TYR
1	C	485	ILE
1	D	514	TYR
1	B	472	ASN

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%)	312 (96%)	14 (4%)	40	51
1	B	316/375 (84%)	308 (98%)	8 (2%)	60	75
1	C	308/375 (82%)	296 (96%)	12 (4%)	43	57
1	D	308/375 (82%)	300 (97%)	8 (3%)	59	73
All	All	1258/1500 (84%)	1216 (97%)	42 (3%)	50	64

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	PHE
1	A	463	SER
1	A	470	LEU
1	A	486	GLU
1	A	499	LEU

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Mol	Chain	Res	Type
1	A	503	LEU
1	A	512	LEU
1	A	634	LEU
1	A	638	ILE
1	A	666	LYS
1	A	688	CYS
1	A	752	HIS
1	A	814	GLN
1	A	852	SER
1	B	487	THR
1	B	505	GLU
1	B	613	GLU
1	B	677	GLU
1	B	752	HIS
1	B	771	ASN
1	B	814	GLN
1	B	828	LYS
1	C	480	LYS
1	C	498	LEU
1	C	499	LEU
1	C	518	ASN
1	C	523	MET
1	C	595	ARG
1	C	617	VAL
1	C	657	MET
1	C	752	HIS
1	C	771	ASN
1	C	788	ASN
1	C	814	GLN
1	D	469	GLN
1	D	595	ARG
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	HIS

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Mol	Chain	Res	Type
1	A	771	ASN
1	A	788	ASN
1	A	814	GLN
1	B	488	HIS
1	B	635	HIS
1	B	771	ASN
1	B	776	ASN
1	C	518	ASN
1	C	552	GLN
1	C	635	HIS
1	C	771	ASN
1	C	788	ASN
1	C	819	GLN
1	D	488	HIS
1	D	552	GLN
1	D	771	ASN
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	102	-	29,29,29	1.35	4 (13%)	45,45,45	0.74	0
3	SIM	A	4	-	32,32,32	2.01	11 (34%)	46,46,46	1.26	6 (13%)
2	ADP	B	101	-	29,29,29	1.44	6 (20%)	45,45,45	0.85	1 (2%)
2	ADP	B	104	-	29,29,29	1.67	7 (24%)	45,45,45	0.85	1 (2%)
3	SIM	B	3	-	32,32,32	1.95	11 (34%)	46,46,46	1.23	6 (13%)
3	SIM	C	1	-	32,32,32	1.96	10 (31%)	46,46,46	1.24	5 (10%)
2	ADP	C	103	-	29,29,29	1.36	4 (13%)	45,45,45	1.00	3 (6%)
3	SIM	C	2	-	32,32,32	1.88	10 (31%)	46,46,46	1.28	7 (15%)
2	ADP	D	105	-	29,29,29	1.54	6 (20%)	45,45,45	1.00	2 (4%)

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	102	-	-	0/16/32/32	0/1/3/3
3	SIM	A	4	-	-	0/26/55/55	0/0/2/2
2	ADP	B	101	-	-	0/16/32/32	0/1/3/3
2	ADP	B	104	-	-	0/16/32/32	0/1/3/3
3	SIM	B	3	-	-	0/26/55/55	0/0/2/2
3	SIM	C	1	-	-	0/26/55/55	0/0/2/2
2	ADP	C	103	-	-	0/16/32/32	0/1/3/3
3	SIM	C	2	-	-	0/26/55/55	0/0/2/2
2	ADP	D	105	-	-	0/16/32/32	0/1/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	ADP	PA-O3A	4.44	1.67	1.59
3	A	4	SIM	C16-C17	4.40	1.55	1.50
3	C	2	SIM	C16-C17	4.37	1.55	1.50
3	C	1	SIM	O1A-C1	4.16	1.37	1.22
3	C	2	SIM	O1A-C1	4.06	1.36	1.22
3	C	1	SIM	C16-C17	4.06	1.55	1.50
3	B	3	SIM	C13-C12	3.99	1.57	1.52
3	B	3	SIM	O1A-C1	3.98	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	SIM	C9-C8	3.95	1.58	1.54
2	D	105	ADP	PA-O3A	3.87	1.66	1.59
3	A	4	SIM	C19-C18	3.81	1.58	1.52
3	C	1	SIM	C13-C12	3.78	1.57	1.52
3	A	4	SIM	C13-C12	3.67	1.57	1.52
3	C	1	SIM	C19-C18	3.66	1.58	1.52
3	A	4	SIM	O1A-C1	3.66	1.35	1.22
3	C	2	SIM	C13-C12	3.60	1.57	1.52
3	B	3	SIM	C9-C8	3.56	1.58	1.54
3	B	3	SIM	C16-C17	3.56	1.54	1.50
3	B	3	SIM	C19-C18	3.53	1.58	1.52
3	C	2	SIM	C19-C18	3.42	1.58	1.52
2	C	103	ADP	C8-N7	-3.10	1.28	1.34
2	D	105	ADP	C8-N7	-3.06	1.28	1.34
2	B	104	ADP	O4'-C1'	2.97	1.45	1.41
2	B	101	ADP	O4'-C4'	2.95	1.51	1.45
2	A	102	ADP	C8-N7	-2.92	1.28	1.34
2	B	104	ADP	C8-N7	-2.90	1.28	1.34
3	C	1	SIM	C9-C8	2.89	1.57	1.54
2	B	101	ADP	C8-N7	-2.87	1.28	1.34
3	C	1	SIM	O14-C18	2.86	1.39	1.34
2	B	104	ADP	O4'-C4'	2.83	1.51	1.45
2	D	105	ADP	O4'-C4'	2.76	1.51	1.45
3	C	2	SIM	C9-C8	2.69	1.57	1.54
2	C	103	ADP	PA-O3A	2.69	1.64	1.59
3	B	3	SIM	C9-C10	2.68	1.55	1.50
2	A	102	ADP	PA-O3A	2.66	1.64	1.59
3	C	1	SIM	C13-C8	2.65	1.58	1.54
3	B	3	SIM	C13-C8	2.62	1.58	1.54
3	C	1	SIM	C9-C10	2.54	1.55	1.50
3	A	4	SIM	O1B-C1	-2.54	1.21	1.30
2	B	101	ADP	C8-N9	-2.49	1.32	1.36
3	C	2	SIM	C9-C10	2.48	1.55	1.50
2	B	101	ADP	PA-O3A	2.48	1.64	1.59
3	A	4	SIM	C13-C8	2.48	1.58	1.54
2	B	104	ADP	C2'-C3'	2.40	1.60	1.53
3	A	4	SIM	C9-C10	2.38	1.54	1.50
3	C	1	SIM	C11-C12	-2.37	1.36	1.43
3	A	4	SIM	O14-C18	2.35	1.38	1.34
2	B	104	ADP	C8-N9	-2.33	1.33	1.36
3	C	2	SIM	O1B-C1	-2.30	1.22	1.30
2	A	102	ADP	C8-N9	-2.27	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	105	ADP	C8-N9	-2.27	1.33	1.36
3	C	2	SIM	C11-C12	-2.25	1.37	1.43
2	A	102	ADP	O4'-C4'	2.24	1.50	1.45
2	B	101	ADP	O4'-C1'	2.22	1.44	1.41
2	C	103	ADP	C8-N9	-2.20	1.33	1.36
3	C	2	SIM	C13-C8	2.18	1.58	1.54
3	A	4	SIM	C11-C12	-2.17	1.37	1.43
3	B	3	SIM	O1B-C1	-2.15	1.22	1.30
2	C	103	ADP	C2'-C3'	2.13	1.59	1.53
3	C	2	SIM	C15-C14	2.12	1.56	1.52
3	A	4	SIM	C15-C14	2.11	1.56	1.52
3	B	3	SIM	C11-C12	-2.09	1.37	1.43
2	D	105	ADP	C1'-N9	2.08	1.55	1.48
2	D	105	ADP	O4'-C1'	2.05	1.44	1.41
3	B	3	SIM	C15-C14	2.05	1.56	1.52
2	B	101	ADP	C2'-C3'	2.02	1.59	1.53
3	C	1	SIM	O1B-C1	-2.02	1.23	1.30
2	B	104	ADP	O2'-C2'	2.01	1.47	1.43
3	B	3	SIM	C11-C10	2.01	1.37	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	ADP	O4'-C1'-N9	4.36	112.50	108.44
3	A	4	SIM	C24-C16-C17	-3.62	108.00	111.25
3	C	2	SIM	C8-C9-C10	-3.42	108.63	110.77
3	B	3	SIM	C24-C16-C17	-3.34	108.25	111.25
3	C	1	SIM	C24-C16-C17	-3.14	108.43	111.25
3	C	2	SIM	O1B-C1-C2	2.93	124.34	114.20
3	C	2	SIM	C9A-C9-C10	-2.93	106.39	110.80
3	C	1	SIM	O1A-C1-C2	-2.90	112.33	122.62
3	C	1	SIM	O1B-C1-C2	2.89	124.20	114.20
3	B	3	SIM	O1B-C1-C2	2.89	124.18	114.20
3	C	2	SIM	C24-C16-C17	-2.88	108.67	111.25
3	C	2	SIM	O1A-C1-C2	-2.85	112.50	122.62
3	A	4	SIM	C9A-C9-C10	-2.84	106.52	110.80
2	C	103	ADP	C4'-O4'-C1'	2.83	112.82	109.75
3	B	3	SIM	O1A-C1-C2	-2.82	112.64	122.62
3	C	1	SIM	C9A-C9-C10	-2.80	106.57	110.80
3	A	4	SIM	O1B-C1-C2	2.77	123.77	114.20
2	B	101	ADP	O4'-C1'-N9	2.69	110.94	108.44
3	C	1	SIM	C8-C9-C10	-2.65	109.11	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	SIM	C8-C9-C10	-2.64	109.12	110.77
3	A	4	SIM	O1A-C1-C2	-2.56	113.55	122.62
3	C	2	SIM	C14-O14-C18	2.53	121.58	117.40
2	B	104	ADP	O4'-C1'-N9	2.51	110.77	108.44
3	B	3	SIM	C9A-C9-C10	-2.49	107.04	110.80
3	B	3	SIM	C8-C9-C10	-2.31	109.33	110.77
3	A	4	SIM	C14-O14-C18	2.20	121.03	117.40
3	B	3	SIM	O14-C14-C15	2.14	112.37	108.00
3	C	2	SIM	C8-C13-C14	-2.14	110.90	114.19
2	C	103	ADP	C3'-C2'-C1'	2.12	104.22	100.91
2	D	105	ADP	N3-C4-N9	2.07	129.16	125.43
2	C	103	ADP	O4'-C1'-N9	-2.05	106.53	108.44

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	408/467 (87%)	1.12	87 (21%) 1 2	36, 57, 100, 101	0
1	B	398/467 (85%)	1.13	80 (20%) 2 3	38, 57, 91, 101	0
1	C	389/467 (83%)	1.04	74 (19%) 2 3	39, 58, 86, 101	0
1	D	388/467 (83%)	0.96	68 (17%) 2 4	36, 54, 83, 101	0
All	All	1583/1868 (84%)	1.06	309 (19%) 2 3	36, 57, 96, 101	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	12.5
1	D	484	LEU	8.8
1	A	484	LEU	8.3
1	A	473	ALA	8.1
1	D	479	TYR	8.1
1	B	476	ILE	7.7
1	A	475	HIS	7.1
1	B	485	ILE	6.7
1	D	485	ILE	6.7
1	C	484	LEU	6.5
1	A	462	LEU	6.4
1	B	471	VAL	6.2
1	A	476	ILE	6.1
1	B	478	ALA	6.1
1	A	479	TYR	6.0
1	B	483	THR	6.0
1	C	627	ARG	5.9
1	B	484	LEU	5.8
1	C	483	THR	5.8
1	C	628	PHE	5.6
1	C	694	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	628	PHE	5.5
1	D	480	LYS	5.5
1	B	477	PRO	5.4
1	D	694	ALA	5.4
1	B	479	TYR	5.4
1	D	745	SER	5.4
1	D	695	ALA	5.4
1	D	467	ILE	5.3
1	A	448	CYS	5.3
1	C	486	GLU	5.3
1	B	630	ARG	5.2
1	D	478	ALA	5.2
1	B	486	GLU	5.2
1	C	480	LYS	5.2
1	B	694	ALA	5.1
1	D	743	ALA	5.1
1	C	479	TYR	5.0
1	D	466	GLU	5.0
1	D	746	ILE	4.9
1	A	748	GLY	4.9
1	A	746	ILE	4.9
1	A	471	VAL	4.8
1	C	743	ALA	4.7
1	D	490	ARG	4.6
1	A	472	ASN	4.6
1	A	523	MET	4.6
1	B	469	GLN	4.6
1	B	746	ILE	4.6
1	A	693	PRO	4.6
1	A	481	LEU	4.5
1	B	693	PRO	4.5
1	C	773	GLY	4.5
1	A	446	GLU	4.5
1	C	518	ASN	4.5
1	A	772	VAL	4.4
1	A	480	LYS	4.3
1	A	482	GLU	4.3
1	B	698	TRP	4.3
1	A	698	TRP	4.2
1	D	748	GLY	4.2
1	D	740	SER	4.2
1	B	743	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	777	CYS	4.1
1	A	470	LEU	4.1
1	D	696	ILE	4.1
1	C	695	ALA	4.1
1	B	608	TRP	4.0
1	B	677	GLU	4.0
1	C	481	LEU	4.0
1	A	624	SER	4.0
1	B	772	VAL	4.0
1	D	698	TRP	4.0
1	A	483	THR	4.0
1	D	772	VAL	4.0
1	A	747	GLY	4.0
1	D	482	GLU	4.0
1	D	693	PRO	4.0
1	B	828	LYS	4.0
1	A	461	PHE	4.0
1	A	699	ILE	3.9
1	C	485	ILE	3.9
1	D	523	MET	3.9
1	B	481	LEU	3.9
1	B	487	THR	3.9
1	D	524	GLY	3.9
1	B	501	LYS	3.9
1	D	747	GLY	3.9
1	A	787	THR	3.8
1	B	467	ILE	3.8
1	A	460	LYS	3.8
1	C	693	PRO	3.8
1	B	475	HIS	3.8
1	D	487	THR	3.8
1	C	769	ALA	3.8
1	A	499	LEU	3.8
1	A	743	ALA	3.7
1	C	745	SER	3.7
1	B	472	ASN	3.7
1	D	469	GLN	3.7
1	D	486	GLU	3.7
1	A	749	TYR	3.7
1	D	749	TYR	3.7
1	C	698	TRP	3.6
1	D	464	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	694	ALA	3.6
1	B	695	ALA	3.6
1	C	741	ALA	3.6
1	C	468	ILE	3.6
1	D	494	ILE	3.6
1	C	699	ILE	3.6
1	C	490	ARG	3.6
1	C	740	SER	3.5
1	D	777	CYS	3.5
1	B	696	ILE	3.5
1	B	470	LEU	3.5
1	B	741	ALA	3.5
1	C	482	GLU	3.5
1	C	772	VAL	3.5
1	D	699	ILE	3.4
1	B	754	ALA	3.4
1	D	771	ASN	3.4
1	C	746	ILE	3.4
1	A	620	GLU	3.4
1	D	741	ALA	3.4
1	B	745	SER	3.4
1	B	744	GLY	3.4
1	C	467	ILE	3.4
1	C	696	ILE	3.4
1	B	748	GLY	3.4
1	A	769	ALA	3.3
1	A	778	ILE	3.3
1	A	621	ALA	3.3
1	B	769	ALA	3.3
1	B	613	GLU	3.3
1	A	689	THR	3.3
1	B	773	GLY	3.3
1	B	776	ASN	3.3
1	B	786	PRO	3.3
1	B	523	MET	3.3
1	B	771	ASN	3.3
1	B	480	LYS	3.2
1	B	688	CYS	3.2
1	B	777	CYS	3.2
1	B	757	VAL	3.2
1	B	474	LYS	3.2
1	B	749	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	761	TYR	3.2
1	C	828	LYS	3.2
1	D	774	SER	3.2
1	B	740	SER	3.2
1	A	771	ASN	3.2
1	C	757	VAL	3.2
1	A	445	ASN	3.1
1	C	548	GLU	3.1
1	C	744	GLY	3.1
1	C	749	TYR	3.1
1	B	468	ILE	3.1
1	C	753	ALA	3.1
1	C	487	THR	3.1
1	A	756	ILE	3.1
1	A	828	LYS	3.1
1	C	516	ASP	3.1
1	D	744	GLY	3.1
1	B	674	TYR	3.0
1	B	758	THR	3.0
1	D	768	ALA	3.0
1	C	771	ASN	3.0
1	C	748	GLY	3.0
1	C	478	ALA	3.0
1	A	477	PRO	3.0
1	C	754	ALA	3.0
1	D	776	ASN	3.0
1	D	689	THR	3.0
1	A	695	ALA	2.9
1	C	775	SER	2.9
1	D	627	ARG	2.9
1	B	473	ALA	2.9
1	A	745	SER	2.9
1	A	744	GLY	2.9
1	C	630	ARG	2.9
1	D	465	ALA	2.9
1	B	753	ALA	2.9
1	C	742	MET	2.9
1	B	778	ILE	2.8
1	D	739	GLY	2.8
1	C	770	GLN	2.8
1	D	753	ALA	2.8
1	C	488	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	773	GLY	2.8
1	D	750	ASN	2.8
1	D	742	MET	2.8
1	A	829	ASP	2.8
1	D	775	SER	2.8
1	A	447	GLU	2.8
1	B	756	ILE	2.7
1	B	775	SER	2.7
1	C	523	MET	2.7
1	C	505	GLU	2.7
1	B	829	ASP	2.7
1	B	620	GLU	2.7
1	D	511	TYR	2.7
1	A	718	ARG	2.6
1	C	521	LEU	2.6
1	B	673	GLU	2.6
1	D	786	PRO	2.6
1	C	616	ALA	2.6
1	D	481	LEU	2.6
1	B	774	SER	2.6
1	A	760	ILE	2.5
1	B	742	MET	2.5
1	C	674	TYR	2.5
1	B	699	ILE	2.5
1	B	747	GLY	2.5
1	A	466	GLU	2.5
1	A	630	ARG	2.5
1	C	777	CYS	2.5
1	C	620	GLU	2.5
1	D	488	HIS	2.5
1	C	464	ASP	2.5
1	B	697	ASN	2.5
1	D	697	ASN	2.5
1	A	510	GLN	2.5
1	A	757	VAL	2.5
1	D	688	CYS	2.5
1	B	762	ILE	2.5
1	C	511	TYR	2.4
1	C	739	GLY	2.4
1	A	738	VAL	2.4
1	D	757	VAL	2.4
1	D	830	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	796	THR	2.4
1	A	514	TYR	2.4
1	A	761	TYR	2.4
1	A	741	ALA	2.4
1	C	465	ALA	2.4
1	A	494	ILE	2.4
1	A	622	PHE	2.4
1	C	768	ALA	2.4
1	B	763	ALA	2.4
1	A	638	ILE	2.4
1	B	689	THR	2.4
1	C	689	THR	2.4
1	C	774	SER	2.4
1	B	629	ALA	2.4
1	C	747	GLY	2.4
1	D	692	LYS	2.4
1	D	769	ALA	2.4
1	B	464	ASP	2.3
1	A	740	SER	2.3
1	B	618	ILE	2.3
1	A	490	ARG	2.3
1	B	768	ALA	2.3
1	B	723	THR	2.3
1	A	696	ILE	2.3
1	A	701	GLY	2.3
1	A	697	ASN	2.3
1	C	789	GLU	2.3
1	C	625	THR	2.3
1	A	773	GLY	2.3
1	D	758	THR	2.3
1	C	622	PHE	2.3
1	A	467	ILE	2.3
1	A	739	GLY	2.3
1	A	750	ASN	2.3
1	D	799	SER	2.3
1	A	444	PRO	2.3
1	A	758	THR	2.3
1	A	608	TRP	2.2
1	C	756	ILE	2.2
1	A	501	LYS	2.2
1	D	737	LEU	2.2
1	C	800	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	742	MET	2.2
1	B	738	VAL	2.2
1	D	738	VAL	2.2
1	B	770	GLN	2.2
1	C	515	ARG	2.2
1	C	718	ARG	2.2
1	A	629	ALA	2.2
1	A	753	ALA	2.2
1	A	715	LYS	2.1
1	B	860	GLY	2.1
1	D	491	GLY	2.1
1	A	759	ALA	2.1
1	B	681	LEU	2.1
1	A	617	VAL	2.1
1	B	692	LYS	2.1
1	D	706	VAL	2.1
1	D	650	ARG	2.1
1	D	666	LYS	2.1
1	A	737	LEU	2.1
1	D	797	MET	2.1
1	A	627	ARG	2.1
1	A	798	PRO	2.1
1	A	754	ALA	2.1
1	B	666	LYS	2.1
1	B	737	LEU	2.1
1	C	499	LEU	2.1
1	D	718	ARG	2.1
1	C	609	LEU	2.0
1	A	474	LYS	2.0
1	A	666	LYS	2.0
1	A	636	THR	2.0
1	B	739	GLY	2.0
1	C	670	LYS	2.0
1	C	832	GLY	2.0
1	C	750	ASN	2.0
1	C	497	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	B	104	27/27	0.36	5.28	99,100,100,100	0
2	ADP	D	105	27/27	0.34	2.86	99,100,100,100	0
2	ADP	C	103	27/27	0.36	1.93	99,100,100,100	0
2	ADP	A	102	27/27	0.31	1.48	100,100,100,100	0
2	ADP	B	101	27/27	0.26	0.73	99,100,100,100	0
3	SIM	C	1	31/31	0.20	0.30	52,60,62,63	0
3	SIM	A	4	31/31	0.19	0.26	59,64,67,67	0
3	SIM	B	3	31/31	0.18	-0.03	50,59,63,63	0
3	SIM	C	2	31/31	0.17	-0.08	51,60,63,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.