



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:15 am GMT

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

This is a Full wwPDB 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

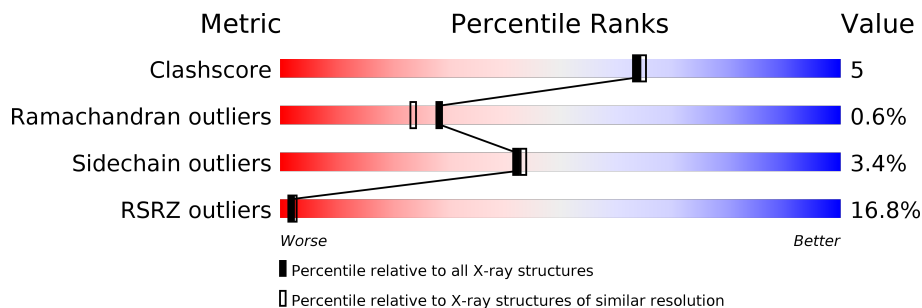
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>16%</div> <div>77%</div> <div>9%</div> <div>13%</div> </div>
1	B	467	<div> <div>15%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	C	467	<div> <div>15%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	D	467	<div> <div>11%</div> <div>73%</div> <div>8%</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12159 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.

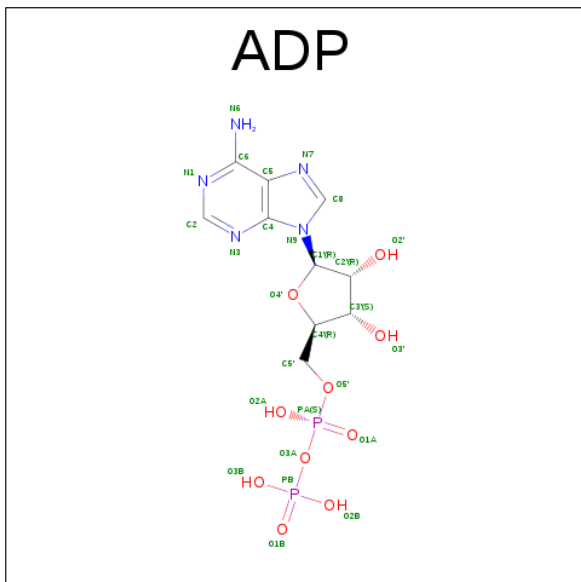
- Molecule 1 is a protein called HMG-COA REDUCTASE.

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

There are 20 discrepancies between the modelled and reference sequences:

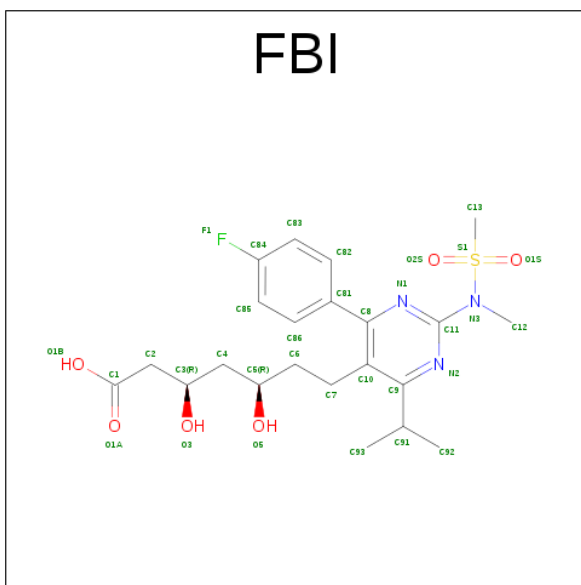
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	INSERTION	UNP P04035
A	423	ALA	-	INSERTION	UNP P04035
A	424	MET	-	INSERTION	UNP P04035
A	425	ALA	-	INSERTION	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	422	GLY	-	INSERTION	UNP P04035
B	423	ALA	-	INSERTION	UNP P04035
B	424	MET	-	INSERTION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

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



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

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



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

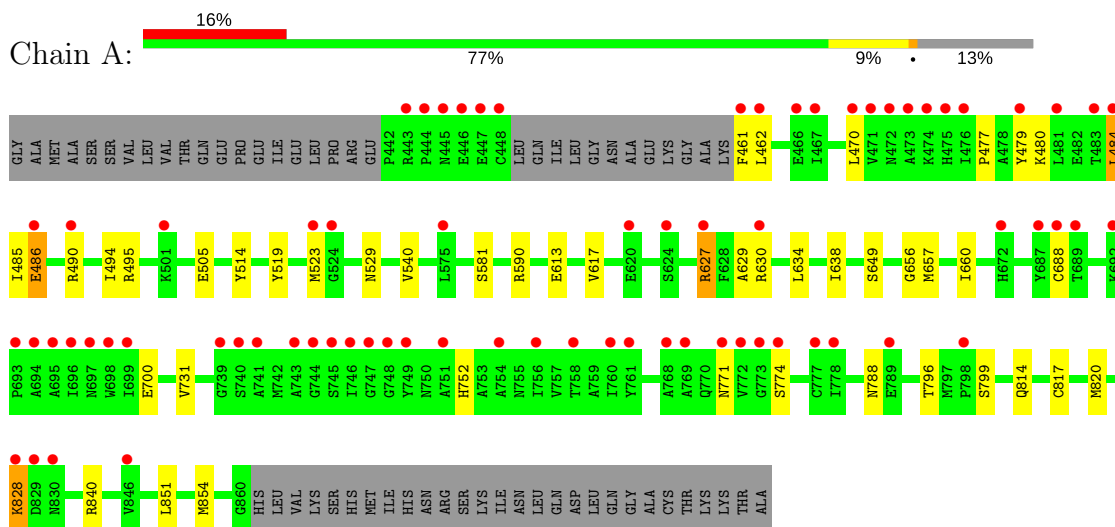
- Molecule 4 is water.

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

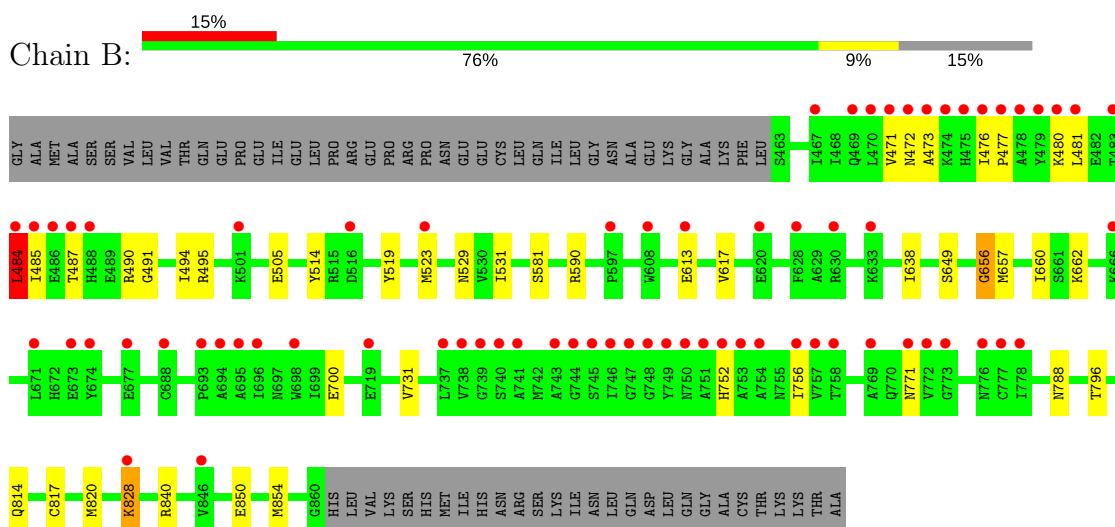
3 Residue-property plots [i](#)

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.

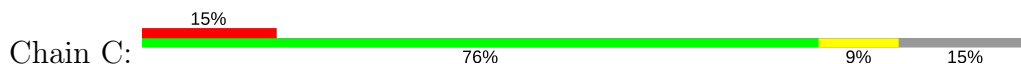
• Molecule 1: HMG-COA REDUCTASE

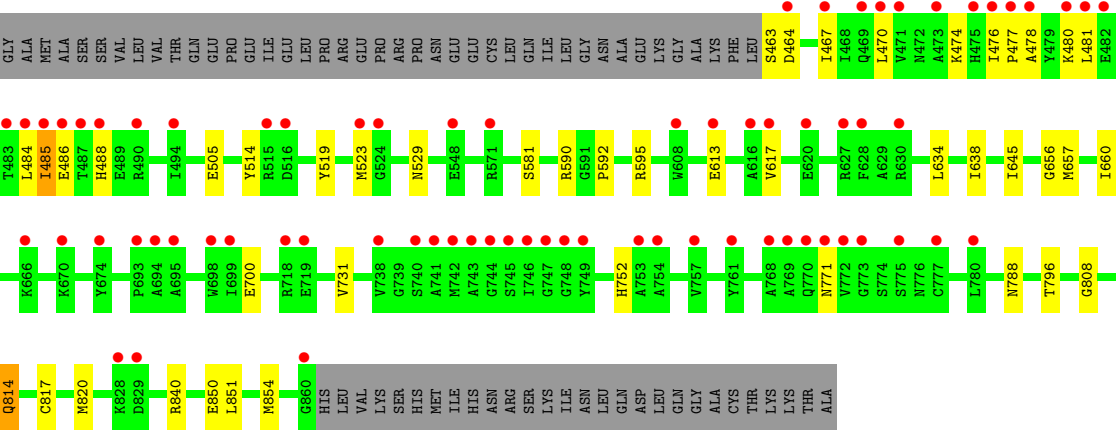


• Molecule 1: HMG-COA REDUCTASE

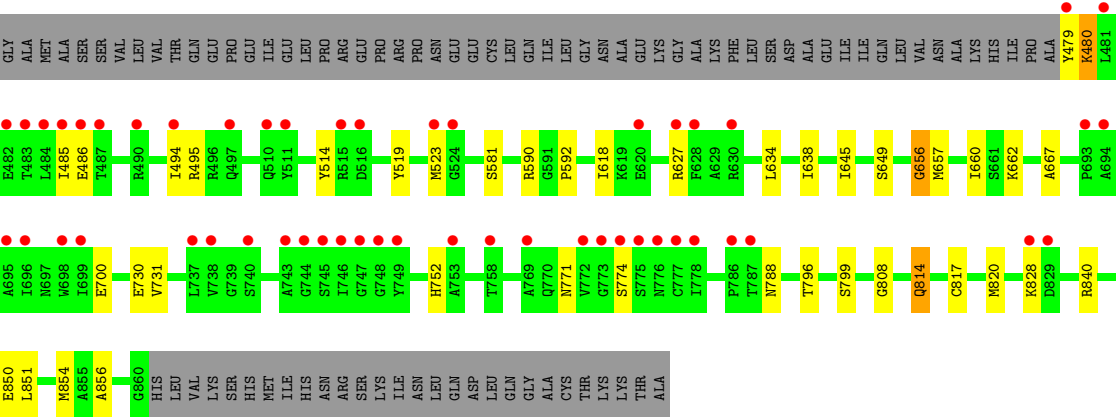


• Molecule 1: HMG-COA REDUCTASE





● 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	74.43Å 172.51Å 79.99Å 90.00° 117.36° 90.00°	Depositor
Resolution (Å)	43.29 – 2.10 43.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.29-2.10) 91.7 (43.29-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.239 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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: FBI, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3072	0.67	0/4153
1	B	0.50	0/2994	0.67	1/4049 (0.0%)
1	C	0.49	0/2994	0.66	0/4049
1	D	0.54	0/2872	0.68	1/3882 (0.0%)
All	All	0.51	0/11932	0.67	2/16133 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 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	3028	0	3059	29	0
1	B	2952	0	2989	33	0
1	C	2952	0	2989	30	0
1	D	2832	0	2865	29	0
2	A	54	0	24	5	0

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

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 5.

All (118) 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:D:523:MET:HE1	4:D:1055:HOH:O	1.69	0.92
1:A:828:LYS:H	1:A:828:LYS:HD2	1.40	0.85
1:B:828:LYS:H	1:B:828:LYS:HD2	1.41	0.85
1:C:485:ILE:HG22	1:C:486:GLU:H	1.44	0.82
1:A:817:CYS:HA	1:A:820:MET:HE3	1.66	0.77
1:C:817:CYS:HA	1:C:820:MET:HE3	1.66	0.77
1:B:817:CYS:HA	1:B:820:MET:HE3	1.67	0.77
1:D:817:CYS:HA	1:D:820:MET:HE3	1.66	0.76
1:A:523:MET:HE1	4:A:1092:HOH:O	1.87	0.75
3:D:3:FBI:H91	3:D:3:FBI:H61	1.69	0.74
3:B:1:FBI:H91	3:B:1:FBI:H61	1.74	0.70
1:A:629:ALA:O	1:A:630:ARG:HD2	1.92	0.69
2:A:102:ADP:H2	1:B:529:ASN:HD22	1.39	0.68
1:B:828:LYS:H	1:B:828:LYS:CD	2.06	0.68
1:C:485:ILE:HG22	1:C:486:GLU:N	2.07	0.68
1:A:828:LYS:H	1:A:828:LYS:CD	2.07	0.68
1:B:523:MET:HE1	4:B:1108:HOH:O	1.95	0.64
2:A:102:ADP:H2	1:B:529:ASN:ND2	1.95	0.63
1:A:485:ILE:HD13	1:A:494:ILE:HD12	1.80	0.63
1:C:523:MET:HE1	4:C:1087:HOH:O	1.99	0.62
1:D:480:LYS:H	1:D:480:LYS:HD3	1.65	0.62
3:A:2:FBI:H61	3:A:2:FBI:H91	1.81	0.62
1:C:519:TYR:O	1:C:523:MET:HG2	2.00	0.62
1:D:519:TYR:O	1:D:523:MET:HG2	2.02	0.60

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:SER:O	1:C:467:ILE:HG12	2.15	0.47
1:C:613:GLU:O	1:C:617:VAL:HG23	2.15	0.47
1:A:627:ARG:HH11	1:A:627:ARG:HG2	1.79	0.46
1:C:820:MET:HE2	1:C:820:MET:HB2	1.80	0.46
1:C:478:ALA:O	1:C:481:LEU:HG	2.16	0.46
1:A:477:PRO:HD2	1:A:480:LYS:HD2	1.97	0.46
1:B:731:VAL:HG12	1:B:854:MET:CE	2.46	0.46
1:A:638:ILE:O	1:D:796:THR:HG21	2.15	0.45
1:D:774:SER:HA	1:D:799:SER:O	2.17	0.45
1:A:731:VAL:HG12	1:A:854:MET:CE	2.46	0.45
1:A:629:ALA:C	1:A:630:ARG:HD2	2.37	0.45
1:B:481:LEU:HD12	1:B:495:ARG:HB2	1.99	0.45
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.84	0.45
1:D:485:ILE:HG22	1:D:486:GLU:H	1.83	0.44
1:D:649:SER:HB3	1:D:660:ILE:HD12	1.98	0.44
1:A:656:GLY:O	1:A:660:ILE:HG12	2.17	0.44
1:A:490:ARG:HD3	1:A:490:ARG:HA	1.73	0.44
1:D:485:ILE:CD1	1:D:494:ILE:HD12	2.48	0.43
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.84	0.43
1:C:592:PRO:HD2	1:C:645:ILE:O	2.17	0.43
1:D:523:MET:HA	1:D:523:MET:CE	2.48	0.43
1:D:820:MET:HB2	1:D:820:MET:HE2	1.81	0.43
1:C:481:LEU:O	1:C:485:ILE:HD12	2.19	0.43
1:D:485:ILE:CG2	1:D:486:GLU:N	2.81	0.43
1:D:662:LYS:HB3	1:D:662:LYS:HE2	1.83	0.42
1:B:638:ILE:O	1:C:796:THR:HG21	2.19	0.42
1:C:488:HIS:CD2	1:C:523:MET:HG3	2.54	0.42
1:A:649:SER:HB3	1:A:660:ILE:HD12	2.02	0.42
1:B:484:LEU:HA	1:B:484:LEU:HD12	1.89	0.42
1:D:592:PRO:HD2	1:D:645:ILE:O	2.20	0.42
1:B:477:PRO:HD2	1:B:480:LYS:HD2	2.01	0.42
1:C:731:VAL:HG12	1:C:854:MET:HE1	2.01	0.42
1:C:595:ARG:HH22	1:D:730:GLU:HG2	1.84	0.42
1:B:485:ILE:HD12	1:B:491:GLY:HA2	2.01	0.42
1:C:808:GLY:O	1:C:814:GLN:HG3	2.20	0.42
1:A:796:THR:HG21	1:D:638:ILE:O	2.20	0.42
1:D:850:GLU:O	1:D:854:MET:HG2	2.19	0.42
1:A:461:PHE:HB3	1:A:462:LEU:HD12	2.03	0.41
1:B:523:MET:HE3	1:B:523:MET:HA	2.01	0.41
1:B:756:ILE:HD12	1:B:756:ILE:N	2.35	0.41
1:C:850:GLU:O	1:C:854:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:HA	1:A:523:MET:CE	2.51	0.41
1:A:540:VAL:CG2	1:B:531:ILE:HD13	2.51	0.41
1:D:618:ILE:HG23	1:D:667:ALA:HB1	2.03	0.41
1:B:662:LYS:HB3	1:B:662:LYS:HE2	1.84	0.41
1:B:649:SER:HB3	1:B:660:ILE:HD12	2.03	0.40
1:B:850:GLU:O	1:B:854:MET:HG2	2.22	0.40
3:C:4:FBI:H3	3:C:4:FBI:H62	1.89	0.40
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.80	0.40
1:A:774:SER:HA	1:A:799:SER:O	2.21	0.40
1:C:474:LYS:HB2	1:C:476:ILE:HG13	2.04	0.40
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.82	0.40
1:D:808:GLY:O	1:D:814:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/467 (86%)	385 (96%)	15 (4%)	3 (1%)	25	20
1	B	396/467 (85%)	376 (95%)	17 (4%)	3 (1%)	22	17
1	C	396/467 (85%)	378 (96%)	16 (4%)	2 (0%)	32	28
1	D	380/467 (81%)	364 (96%)	15 (4%)	1 (0%)	44	44
All	All	1575/1868 (84%)	1503 (95%)	63 (4%)	9 (1%)	28	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	472	ASN
1	B	484	LEU
1	A	484	LEU

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Mol	Chain	Res	Type
1	A	486	GLU
1	D	514	TYR
1	A	514	TYR
1	B	514	TYR
1	C	514	TYR
1	C	485	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/375 (87%)	311 (96%)	14 (4%)	33	32
1	B	316/375 (84%)	308 (98%)	8 (2%)	53	57
1	C	316/375 (84%)	305 (96%)	11 (4%)	41	42
1	D	303/375 (81%)	293 (97%)	10 (3%)	43	45
All	All	1260/1500 (84%)	1217 (97%)	43 (3%)	42	43

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

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

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

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

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

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Mol	Chain	Res	Type
1	D	788	ASN
1	D	830	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	101	-	25,29,29	1.24	2 (8%)	24,45,45	0.79	0
2	ADP	A	102	-	25,29,29	1.23	2 (8%)	24,45,45	0.82	0
3	FBI	A	2	-	29,34,34	3.50	6 (20%)	36,49,49	2.14	7 (19%)
3	FBI	B	1	-	29,34,34	3.41	8 (27%)	36,49,49	2.21	7 (19%)
2	ADP	C	103	-	25,29,29	1.34	4 (16%)	24,45,45	1.08	2 (8%)
3	FBI	C	4	-	29,34,34	3.52	8 (27%)	36,49,49	2.28	8 (22%)
3	FBI	D	3	-	29,34,34	3.42	6 (20%)	36,49,49	2.13	8 (22%)

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	FBI	A	2	-	-	0/29/31/31	0/2/2/2
3	FBI	B	1	-	-	0/29/31/31	0/2/2/2
2	ADP	C	103	-	-	0/12/32/32	0/3/3/3
3	FBI	C	4	-	-	0/29/31/31	0/2/2/2
3	FBI	D	3	-	-	0/29/31/31	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FBI	C81-C8	-9.55	1.38	1.49
3	B	1	FBI	C81-C8	-9.09	1.39	1.49
3	D	3	FBI	C81-C8	-9.00	1.39	1.49
3	A	2	FBI	C81-C8	-8.97	1.39	1.49
3	C	4	FBI	C6-C7	-4.41	1.32	1.53
3	D	3	FBI	C6-C7	-4.28	1.33	1.53
3	A	2	FBI	C6-C7	-4.13	1.33	1.53
3	B	1	FBI	C6-C7	-4.10	1.33	1.53
2	C	103	ADP	C8-N7	-3.63	1.27	1.34
2	A	102	ADP	C8-N7	-3.36	1.28	1.34
2	A	101	ADP	C8-N7	-3.35	1.28	1.34
3	C	4	FBI	C11-N2	-2.29	1.30	1.34
2	C	103	ADP	PB-O3A	-2.29	1.56	1.60
3	B	1	FBI	C11-N1	-2.00	1.31	1.34
2	A	102	ADP	O4'-C4'	2.01	1.49	1.45
3	C	4	FBI	C83-C84	2.05	1.41	1.37
3	B	1	FBI	C83-C84	2.09	1.41	1.37
2	C	103	ADP	O4'-C4'	2.21	1.50	1.45
2	C	103	ADP	C2'-C3'	2.24	1.59	1.53
3	C	4	FBI	C7-C10	2.31	1.55	1.52
2	A	101	ADP	O4'-C4'	2.56	1.50	1.45
3	A	2	FBI	C8-C10	2.58	1.45	1.41
3	B	1	FBI	C8-C10	2.84	1.45	1.41
3	D	3	FBI	C10-C9	2.94	1.45	1.41
3	B	1	FBI	C9-C91	3.97	1.56	1.51
3	C	4	FBI	C9-C91	4.20	1.56	1.51
3	A	2	FBI	C9-C91	4.24	1.56	1.51
3	D	3	FBI	C9-C91	4.83	1.57	1.51
3	C	4	FBI	O2S-S1	9.36	1.59	1.43
3	B	1	FBI	O2S-S1	9.37	1.59	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	FBI	O1S-S1	9.55	1.59	1.43
3	D	3	FBI	O1S-S1	9.63	1.59	1.43
3	A	2	FBI	O2S-S1	9.68	1.59	1.43
3	D	3	FBI	O2S-S1	9.69	1.59	1.43
3	C	4	FBI	O1S-S1	10.20	1.60	1.43
3	A	2	FBI	O1S-S1	10.35	1.60	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	FBI	O2S-S1-O1S	-7.97	106.86	118.61
3	C	4	FBI	O2S-S1-O1S	-7.94	106.90	118.61
3	A	2	FBI	O2S-S1-O1S	-7.21	107.98	118.61
3	D	3	FBI	O2S-S1-O1S	-7.08	108.18	118.61
3	C	4	FBI	C10-C8-N1	-3.17	118.50	122.78
3	B	1	FBI	C10-C8-N1	-2.92	118.85	122.78
3	D	3	FBI	C10-C8-N1	-2.83	118.97	122.78
3	A	2	FBI	C10-C8-N1	-2.74	119.09	122.78
3	D	3	FBI	O2S-S1-N3	2.11	109.83	107.09
3	D	3	FBI	C92-C91-C9	2.23	115.11	111.21
2	C	103	ADP	C2'-C3'-C4'	2.32	107.14	102.62
3	C	4	FBI	C82-C81-C8	2.44	124.43	120.59
3	A	2	FBI	O1S-S1-N3	2.55	110.42	107.09
2	C	103	ADP	C4'-O4'-C1'	3.00	112.96	109.77
3	C	4	FBI	O2S-S1-N3	3.08	111.10	107.09
3	C	4	FBI	C11-N2-C9	3.15	119.94	116.24
3	B	1	FBI	O1S-S1-N3	3.17	111.22	107.09
3	D	3	FBI	C11-N2-C9	3.24	120.05	116.24
3	C	4	FBI	O1S-S1-N3	3.29	111.38	107.09
3	B	1	FBI	O2S-S1-N3	3.55	111.72	107.09
3	B	1	FBI	C7-C6-C5	3.61	122.19	115.31
3	A	2	FBI	C11-N2-C9	3.62	120.49	116.24
3	B	1	FBI	C11-N2-C9	3.73	120.62	116.24
3	D	3	FBI	C7-C6-C5	3.87	122.70	115.31
3	A	2	FBI	O2S-S1-N3	3.91	112.18	107.09
3	A	2	FBI	C7-C6-C5	4.00	122.94	115.31
3	C	4	FBI	C6-C7-C10	4.82	125.54	112.11
3	D	3	FBI	O1S-S1-N3	4.84	113.39	107.09
3	D	3	FBI	C6-C7-C10	5.02	126.10	112.11
3	C	4	FBI	C7-C6-C5	5.04	124.93	115.31
3	A	2	FBI	C6-C7-C10	5.09	126.31	112.11
3	B	1	FBI	C6-C7-C10	5.71	128.02	112.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	ADP	2	0
2	A	102	ADP	3	0
3	A	2	FBI	2	0
3	B	1	FBI	2	0
2	C	103	ADP	2	0
3	C	4	FBI	2	0
3	D	3	FBI	2	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	407/467 (87%)	0.87	73 (17%) 2 2	35, 52, 90, 97	0
1	B	398/467 (85%)	0.87	71 (17%) 2 2	35, 52, 82, 100	0
1	C	398/467 (85%)	0.84	72 (18%) 1 2	36, 54, 89, 99	0
1	D	382/467 (81%)	0.70	51 (13%) 4 5	35, 50, 75, 100	0
All	All	1585/1868 (84%)	0.82	267 (16%) 2 2	35, 52, 87, 100	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	9.7
1	A	484	LEU	8.9
1	D	484	LEU	7.7
1	C	475	HIS	7.5
1	A	473	ALA	7.2
1	A	475	HIS	6.6
1	D	479	TYR	6.5
1	B	484	LEU	6.4
1	D	485	ILE	6.0
1	C	484	LEU	6.0
1	C	483	THR	5.9
1	B	481	LEU	5.9
1	B	477	PRO	5.6
1	A	476	ILE	5.6
1	A	471	VAL	5.6
1	A	483	THR	5.5
1	D	746	ILE	5.5
1	C	485	ILE	5.4
1	B	475	HIS	5.3
1	B	476	ILE	5.2
1	A	772	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	486	GLU	5.2
1	B	478	ALA	5.1
1	B	746	ILE	5.0
1	C	470	LEU	4.9
1	A	746	ILE	4.9
1	A	448	CYS	4.8
1	B	486	GLU	4.8
1	B	485	ILE	4.8
1	B	630	ARG	4.8
1	D	694	ALA	4.7
1	A	446	GLU	4.6
1	B	470	LEU	4.6
1	C	486	GLU	4.6
1	C	471	VAL	4.5
1	A	470	LEU	4.4
1	C	674	TYR	4.4
1	A	694	ALA	4.4
1	B	471	VAL	4.4
1	B	469	GLN	4.3
1	D	481	LEU	4.2
1	C	627	ARG	4.2
1	D	627	ARG	4.2
1	D	772	VAL	4.1
1	D	524	GLY	4.0
1	D	516	ASP	4.0
1	B	693	PRO	3.9
1	A	699	ILE	3.9
1	B	694	ALA	3.9
1	C	741	ALA	3.9
1	C	772	VAL	3.8
1	D	695	ALA	3.8
1	B	749	TYR	3.8
1	A	467	ILE	3.8
1	A	777	CYS	3.8
1	C	694	ALA	3.8
1	D	523	MET	3.7
1	C	515	ARG	3.7
1	B	479	TYR	3.7
1	D	828	LYS	3.6
1	A	461	PHE	3.6
1	B	754	ALA	3.6
1	A	698	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	777	CYS	3.6
1	A	769	ALA	3.6
1	D	743	ALA	3.6
1	C	746	ILE	3.6
1	D	482	GLU	3.6
1	C	467	ILE	3.5
1	C	628	PHE	3.5
1	C	523	MET	3.5
1	A	828	LYS	3.5
1	C	773	GLY	3.5
1	D	699	ILE	3.5
1	A	744	GLY	3.5
1	C	476	ILE	3.4
1	A	466	GLU	3.4
1	C	769	ALA	3.4
1	B	483	THR	3.4
1	B	467	ILE	3.4
1	C	695	ALA	3.3
1	B	480	LYS	3.3
1	A	778	ILE	3.3
1	D	745	SER	3.3
1	B	698	TRP	3.3
1	C	718	ARG	3.3
1	B	772	VAL	3.3
1	D	744	GLY	3.3
1	A	474	LYS	3.3
1	C	477	PRO	3.3
1	B	741	ALA	3.3
1	A	479	TYR	3.2
1	A	741	ALA	3.2
1	B	620	GLU	3.2
1	A	630	ARG	3.2
1	C	740	SER	3.2
1	D	696	ILE	3.2
1	C	473	ALA	3.2
1	C	753	ALA	3.2
1	B	487	THR	3.2
1	C	487	THR	3.2
1	D	747	GLY	3.2
1	C	743	ALA	3.1
1	A	627	ARG	3.1
1	C	749	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	695	ALA	3.1
1	A	773	GLY	3.1
1	B	756	ILE	3.1
1	C	757	VAL	3.1
1	D	693	PRO	3.1
1	A	462	LEU	3.1
1	B	757	VAL	3.1
1	A	689	THR	3.1
1	A	481	LEU	3.1
1	A	748	GLY	3.0
1	B	743	ALA	3.0
1	C	745	SER	3.0
1	B	523	MET	3.0
1	A	693	PRO	3.0
1	B	758	THR	3.0
1	B	748	GLY	3.0
1	A	447	GLU	3.0
1	C	698	TRP	3.0
1	A	749	TYR	3.0
1	B	474	LYS	2.9
1	A	472	ASN	2.9
1	C	742	MET	2.9
1	A	754	ALA	2.9
1	A	745	SER	2.9
1	C	699	ILE	2.9
1	B	778	ILE	2.9
1	C	608	TRP	2.9
1	D	490	ARG	2.8
1	B	740	SER	2.8
1	A	443	ARG	2.8
1	A	486	GLU	2.8
1	A	829	ASP	2.8
1	C	482	GLU	2.8
1	C	524	GLY	2.8
1	D	487	THR	2.8
1	B	473	ALA	2.7
1	D	748	GLY	2.7
1	D	630	ARG	2.7
1	D	698	TRP	2.7
1	B	516	ASP	2.7
1	C	478	ALA	2.7
1	A	696	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	829	ASP	2.7
1	C	693	PRO	2.7
1	D	511	TYR	2.7
1	B	828	LYS	2.7
1	B	613	GLU	2.7
1	C	829	ASP	2.7
1	D	758	THR	2.7
1	C	548	GLU	2.6
1	C	747	GLY	2.6
1	C	490	ARG	2.6
1	C	754	ALA	2.6
1	A	771	ASN	2.6
1	A	672	HIS	2.6
1	C	744	GLY	2.6
1	D	777	CYS	2.6
1	A	798	PRO	2.6
1	C	738	VAL	2.6
1	D	749	TYR	2.6
1	D	778	ILE	2.6
1	A	501	LYS	2.6
1	D	786	PRO	2.6
1	A	760	ILE	2.6
1	B	677	GLU	2.6
1	A	740	SER	2.6
1	A	524	GLY	2.6
1	A	688	CYS	2.6
1	B	737	LEU	2.6
1	A	695	ALA	2.5
1	B	753	ALA	2.5
1	D	753	ALA	2.5
1	A	743	ALA	2.5
1	A	697	ASN	2.5
1	C	719	GLU	2.5
1	C	469	GLN	2.5
1	D	515	ARG	2.5
1	D	775	SER	2.5
1	C	771	ASN	2.5
1	D	773	GLY	2.5
1	A	444	PRO	2.5
1	C	770	GLN	2.5
1	B	674	TYR	2.5
1	A	756	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	737	LEU	2.4
1	A	846	VAL	2.4
1	A	830	ASN	2.4
1	C	464	ASP	2.4
1	A	523	MET	2.4
1	A	758	THR	2.4
1	C	670	LYS	2.4
1	C	777	CYS	2.4
1	B	744	GLY	2.4
1	A	620	GLU	2.4
1	C	666	LYS	2.4
1	D	494	ILE	2.4
1	A	687	TYR	2.4
1	B	745	SER	2.4
1	C	761	TYR	2.4
1	C	616	ALA	2.4
1	B	773	GLY	2.4
1	D	740	SER	2.3
1	A	747	GLY	2.3
1	C	488	HIS	2.3
1	D	628	PHE	2.3
1	C	775	SER	2.3
1	C	480	LYS	2.3
1	C	768	ALA	2.3
1	B	488	HIS	2.3
1	B	628	PHE	2.3
1	B	769	ALA	2.3
1	B	846	VAL	2.3
1	B	719	GLU	2.3
1	A	575	LEU	2.2
1	B	750	ASN	2.2
1	B	688	CYS	2.2
1	B	673	GLU	2.2
1	B	738	VAL	2.2
1	B	696	ILE	2.2
1	B	751	ALA	2.2
1	C	481	LEU	2.2
1	C	571	ARG	2.2
1	C	748	GLY	2.2
1	A	761	TYR	2.2
1	D	787	THR	2.2
1	C	617	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	624	SER	2.1
1	B	671	LEU	2.1
1	B	633	LYS	2.1
1	B	747	GLY	2.1
1	B	666	LYS	2.1
1	B	776	ASN	2.1
1	C	620	GLU	2.1
1	C	494	ILE	2.1
1	A	774	SER	2.1
1	A	751	ALA	2.1
1	D	769	ALA	2.1
1	B	608	TRP	2.1
1	B	752	HIS	2.1
1	A	692	LYS	2.1
1	C	516	ASP	2.1
1	D	497	GLN	2.1
1	A	739	GLY	2.1
1	B	739	GLY	2.1
1	C	613	GLU	2.0
1	D	620	GLU	2.0
1	A	445	ASN	2.0
1	A	490	ARG	2.0
1	B	771	ASN	2.0
1	C	630	ARG	2.0
1	D	510	GLN	2.0
1	A	768	ALA	2.0
1	C	860	GLY	2.0
1	D	774	SER	2.0
1	D	776	ASN	2.0
1	B	501	LYS	2.0
1	B	597	PRO	2.0
1	C	828	LYS	2.0
1	A	789	GLU	2.0
1	B	472	ASN	2.0
1	C	780	LEU	2.0
1	D	738	VAL	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 [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	C	103	27/27	0.78	0.25	1.22	83,88,99,99	0
2	ADP	A	101	27/27	0.75	0.26	1.05	90,93,99,99	0
2	ADP	A	102	27/27	0.79	0.26	0.72	88,91,99,99	0
3	FBI	C	4	33/33	0.93	0.14	-0.27	44,51,57,57	0
3	FBI	D	3	33/33	0.91	0.13	-0.35	44,51,57,58	0
3	FBI	B	1	33/33	0.93	0.13	-0.47	46,54,59,59	0
3	FBI	A	2	33/33	0.93	0.14	-0.66	41,48,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.