



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:56 PM GMT

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

This is a Full wwPDB 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

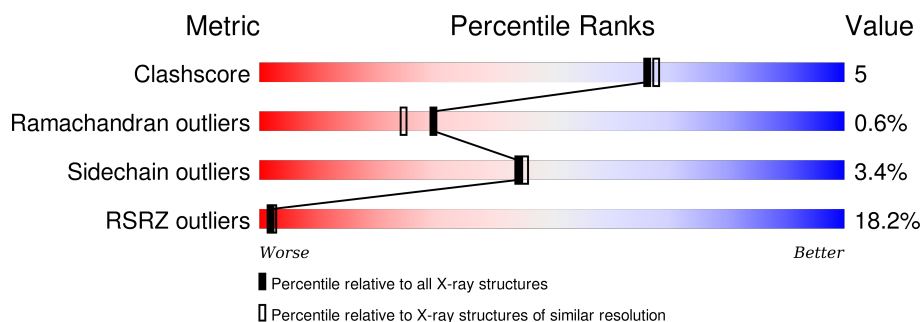
1 Overall quality at a glance

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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	
1	B	467	
1	C	467	
1	D	467	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12159 atoms, of which 0 are 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.

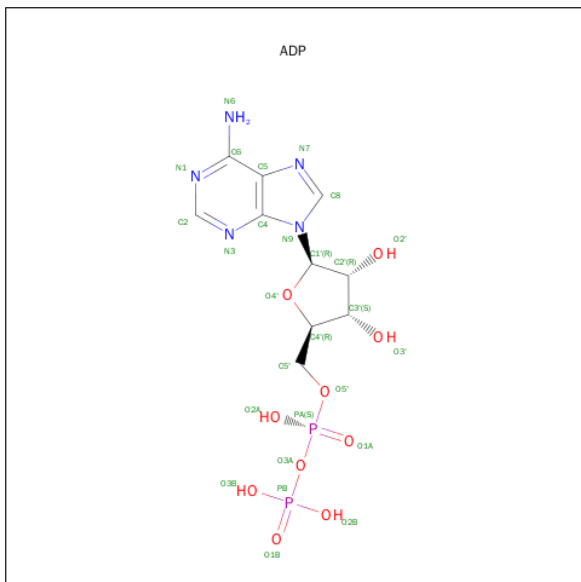
- Molecule 1 is a protein called HMG-COA REDUCTASE.

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:

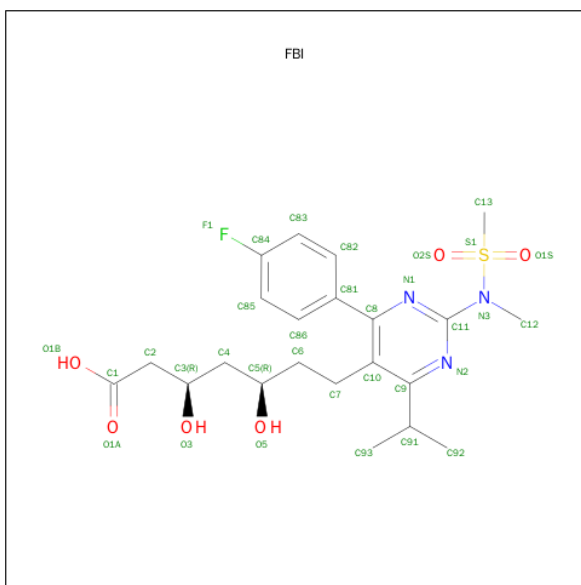
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	INSERTION	UNP P04035
A	423	ALA	-	INSERTION	UNP P04035
A	424	MET	-	INSERTION	UNP P04035
A	425	ALA	-	INSERTION	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	422	GLY	-	INSERTION	UNP P04035
B	423	ALA	-	INSERTION	UNP P04035
B	424	MET	-	INSERTION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

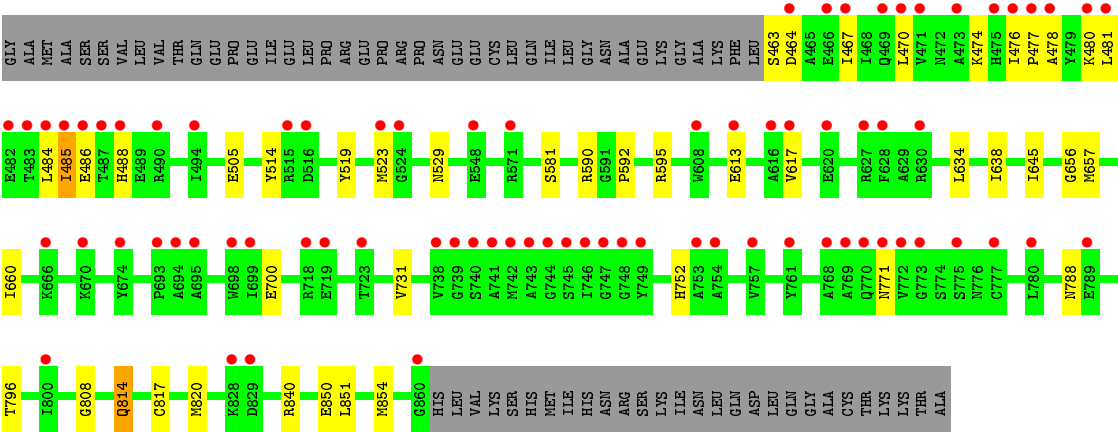
- Molecule 3 is 7-[4-(4-FLUORO-PHENYL)-6-ISOPROPYL-2-(METHANESULFONYL-METHYL-AMINO)-PYRIMIDIN-5-YL]-3,5-DIHYDROXY-HEPTANOIC ACID (three-letter code: FBI) (formula: $C_{22}H_{30}FN_3O_6S$).



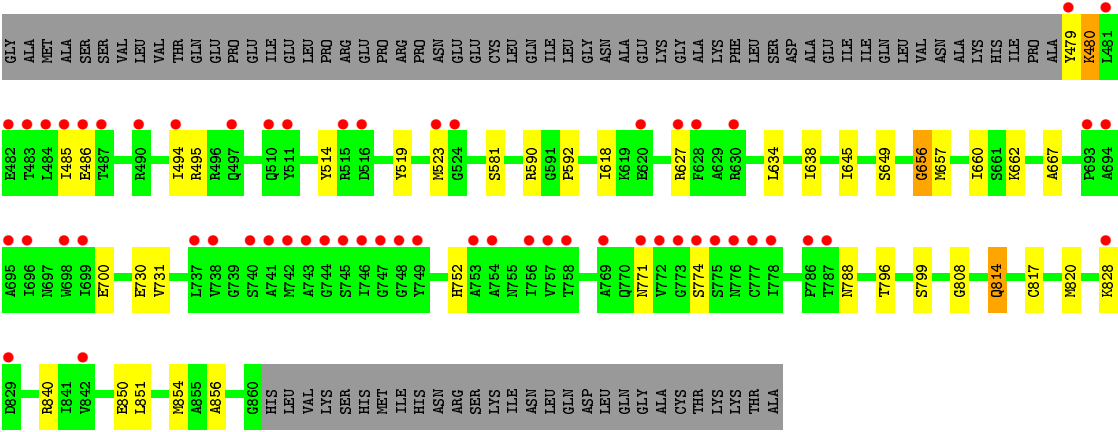
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 33	C 22	F 1	N 3	O 6	S 1	0	0
3	A	1	Total 33	C 22	F 1	N 3	O 6	S 1	0	0
3	D	1	Total 33	C 22	F 1	N 3	O 6	S 1	0	0
3	C	1	Total 33	C 22	F 1	N 3	O 6	S 1	0	0

- Molecule 4 is water.

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



• 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
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101827 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

Continued on next page...

Continued from previous page...

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:H61	3:B:1:FBI:H91	1.74	0.70
1:A:629:ALA:O	1:A:630:ARG:HD2	1.92	0.69
2:A:102:ADP:H2	1:B:529:ASN:HD22	1.39	0.68
1:B:828:LYS:H	1:B:828:LYS:CD	2.06	0.68
1:C:485:ILE:HG22	1:C:486:GLU:N	2.07	0.68
1:A:828:LYS:H	1:A:828:LYS:CD	2.07	0.68
1:B:523:MET:HE1	4:B:1108:HOH:O	1.95	0.64
2:A:102:ADP:H2	1:B:529:ASN:ND2	1.95	0.63
1:A:485:ILE:HD13	1:A:494:ILE:HD12	1.80	0.63
1:C:523:MET:HE1	4:C:1087:HOH:O	1.99	0.62
1:D:480:LYS:H	1:D:480:LYS:HD3	1.65	0.62
3:A:2:FBI:H61	3:A:2:FBI:H91	1.81	0.62
1:C:519:TYR:O	1:C:523:MET:HG2	2.00	0.62
1:D:519:TYR:O	1:D:523:MET:HG2	2.02	0.60

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
3:C:4:FBI:H3	3:C:4:FBI:H62	1.89	0.40
1:B:850:GLU:O	1:B:854:MET:HG2	2.22	0.40
1:C:474:LYS:HB2	1:C:476:ILE:HG13	2.04	0.40
1:D:808:GLY:O	1:D:814:GLN:HG3	2.21	0.40
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.80	0.40
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.82	0.40
1:A:774:SER:HA	1:A:799:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	26	21
1	B	396/467 (85%)	376 (95%)	17 (4%)	3 (1%)	24	17
1	C	396/467 (85%)	378 (96%)	16 (4%)	2 (0%)	34	30
1	D	380/467 (81%)	364 (96%)	15 (4%)	1 (0%)	46	45
All	All	1575/1868 (84%)	1503 (95%)	63 (4%)	9 (1%)	30	24

All (9) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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%)	35	34
1	B	316/375 (84%)	308 (98%)	8 (2%)	55	59
1	C	316/375 (84%)	305 (96%)	11 (4%)	43	44
1	D	303/375 (81%)	293 (97%)	10 (3%)	45	47
All	All	1260/1500 (84%)	1217 (97%)	43 (3%)	44	45

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	-	22,29,29	1.27	2 (9%)	27,45,45	0.68	0
2	ADP	A	102	-	22,29,29	1.27	1 (4%)	27,45,45	0.76	0
3	FBI	A	2	-	31,34,34	4.69	8 (25%)	36,49,49	2.27	9 (25%)
3	FBI	B	1	-	31,34,34	4.44	9 (29%)	36,49,49	2.33	8 (22%)
2	ADP	C	103	-	22,29,29	1.32	3 (13%)	27,45,45	1.00	2 (7%)
3	FBI	C	4	-	31,34,34	4.60	11 (35%)	36,49,49	2.37	9 (25%)
3	FBI	D	3	-	31,34,34	4.48	9 (29%)	36,49,49	2.27	9 (25%)

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	-	-	0/27/31/31	0/2/2/2
3	FBI	B	1	-	-	0/27/31/31	0/2/2/2
2	ADP	C	103	-	-	0/12/32/32	0/3/3/3
3	FBI	C	4	-	-	0/27/31/31	0/2/2/2
3	FBI	D	3	-	-	0/27/31/31	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FBI	C81-C8	-9.32	1.38	1.49
3	B	1	FBI	C81-C8	-8.86	1.39	1.49
3	D	3	FBI	C81-C8	-8.77	1.39	1.49
3	A	2	FBI	C81-C8	-8.74	1.39	1.49
3	C	4	FBI	C6-C7	-4.21	1.32	1.52
3	D	3	FBI	C6-C7	-4.09	1.33	1.52
3	A	2	FBI	C6-C7	-3.94	1.33	1.52
3	B	1	FBI	C6-C7	-3.92	1.33	1.52
2	C	103	ADP	C8-N7	-3.51	1.27	1.34
2	A	102	ADP	C8-N7	-3.25	1.28	1.34
2	A	101	ADP	C8-N7	-3.24	1.28	1.34
3	C	4	FBI	C11-N2	-2.25	1.30	1.34
3	C	4	FBI	C83-C84	2.02	1.41	1.37
3	B	1	FBI	C83-C84	2.06	1.41	1.37
2	C	103	ADP	O4'-C4'	2.16	1.50	1.45
2	C	103	ADP	C2'-C3'	2.19	1.59	1.53
3	C	4	FBI	C8-C10	2.26	1.44	1.40
3	C	4	FBI	C7-C10	2.29	1.55	1.52
3	D	3	FBI	C8-C10	2.32	1.44	1.40
2	A	101	ADP	O4'-C4'	2.50	1.50	1.45
3	D	3	FBI	C10-C9	2.86	1.45	1.41
3	A	2	FBI	C8-C10	3.13	1.45	1.40
3	B	1	FBI	S1-N3	3.14	1.72	1.65
3	B	1	FBI	C8-C10	3.42	1.45	1.40
3	B	1	FBI	C9-C91	3.86	1.56	1.51
3	C	4	FBI	S1-N3	3.88	1.74	1.65
3	D	3	FBI	S1-N3	4.02	1.74	1.65
3	C	4	FBI	C9-C91	4.08	1.56	1.51
3	A	2	FBI	C9-C91	4.12	1.56	1.51
3	A	2	FBI	S1-N3	4.20	1.74	1.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	FBI	C11-N3	4.47	1.45	1.37
3	D	3	FBI	C9-C91	4.67	1.57	1.51
3	B	1	FBI	C11-N3	5.05	1.46	1.37
3	C	4	FBI	C11-N3	5.42	1.46	1.37
3	A	2	FBI	C11-N3	6.48	1.48	1.37
3	C	4	FBI	O2S-S1	14.36	1.59	1.43
3	B	1	FBI	O2S-S1	14.38	1.59	1.43
3	B	1	FBI	O1S-S1	14.65	1.59	1.43
3	D	3	FBI	O1S-S1	14.78	1.59	1.43
3	A	2	FBI	O2S-S1	14.86	1.59	1.43
3	D	3	FBI	O2S-S1	14.87	1.59	1.43
3	C	4	FBI	O1S-S1	15.65	1.60	1.43
3	A	2	FBI	O1S-S1	15.87	1.60	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	FBI	O2S-S1-O1S	-8.48	106.86	118.66
3	C	4	FBI	O2S-S1-O1S	-8.45	106.90	118.66
3	A	2	FBI	O2S-S1-O1S	-7.68	107.98	118.66
3	D	3	FBI	O2S-S1-O1S	-7.54	108.18	118.66
3	D	3	FBI	C10-C9-N2	-4.60	118.90	123.11
3	A	2	FBI	C10-C9-N2	-4.27	119.20	123.11
3	B	1	FBI	C10-C9-N2	-4.20	119.27	123.11
3	C	4	FBI	C10-C9-N2	-3.62	119.81	123.11
3	C	4	FBI	C10-C8-N1	-3.12	118.50	122.73
3	B	1	FBI	C10-C8-N1	-2.87	118.85	122.73
3	D	3	FBI	C10-C8-N1	-2.78	118.97	122.73
3	A	2	FBI	C10-C8-N1	-2.69	119.09	122.73
3	D	3	FBI	C92-C91-C9	2.14	115.11	111.26
3	A	2	FBI	C91-C9-N2	2.15	117.51	115.68
2	C	103	ADP	C2'-C3'-C4'	2.20	107.14	102.61
3	D	3	FBI	O2S-S1-N3	2.23	109.83	106.94
3	C	4	FBI	C82-C81-C8	2.45	124.43	120.60
3	A	2	FBI	O1S-S1-N3	2.68	110.42	106.94
3	C	4	FBI	C11-N2-C9	2.89	119.94	116.31
2	C	103	ADP	C4'-O4'-C1'	2.95	112.96	109.72
3	D	3	FBI	C11-N2-C9	2.98	120.05	116.31
3	C	4	FBI	O2S-S1-N3	3.21	111.10	106.94
3	B	1	FBI	O1S-S1-N3	3.30	111.22	106.94
3	A	2	FBI	C11-N2-C9	3.33	120.49	116.31
3	B	1	FBI	C7-C6-C5	3.34	122.19	115.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FBI	O1S-S1-N3	3.42	111.38	106.94
3	B	1	FBI	C11-N2-C9	3.43	120.62	116.31
3	D	3	FBI	C7-C6-C5	3.58	122.70	115.31
3	B	1	FBI	O2S-S1-N3	3.68	111.72	106.94
3	A	2	FBI	C7-C6-C5	3.70	122.94	115.31
3	A	2	FBI	O2S-S1-N3	4.03	112.18	106.94
3	C	4	FBI	C6-C7-C10	4.55	125.54	111.94
3	C	4	FBI	C7-C6-C5	4.66	124.93	115.31
3	D	3	FBI	C6-C7-C10	4.73	126.10	111.94
3	A	2	FBI	C6-C7-C10	4.80	126.31	111.94
3	D	3	FBI	O1S-S1-N3	4.97	113.39	106.94
3	B	1	FBI	C6-C7-C10	5.37	128.02	111.94

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%)	0.95	80 (19%) 1 2	35, 52, 90, 97	0
1	B	398/467 (85%)	0.95	74 (18%) 2 2	35, 52, 82, 100	0
1	C	398/467 (85%)	0.93	77 (19%) 2 2	36, 54, 89, 99	0
1	D	382/467 (81%)	0.78	58 (15%) 3 4	35, 50, 75, 100	0
All	All	1585/1868 (84%)	0.90	289 (18%) 2 2	35, 52, 87, 100	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	10.1
1	A	484	LEU	9.3
1	D	484	LEU	8.0
1	C	475	HIS	7.7
1	A	473	ALA	7.6
1	A	475	HIS	6.8
1	B	484	LEU	6.7
1	D	479	TYR	6.7
1	D	485	ILE	6.4
1	C	484	LEU	6.3
1	B	481	LEU	6.2
1	C	483	THR	6.2
1	A	476	ILE	5.9
1	A	471	VAL	5.9
1	B	477	PRO	5.8
1	D	746	ILE	5.8
1	A	483	THR	5.7
1	C	485	ILE	5.7
1	A	772	VAL	5.6
1	B	476	ILE	5.6
1	B	475	HIS	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	486	GLU	5.4
1	B	478	ALA	5.4
1	B	746	ILE	5.3
1	A	746	ILE	5.2
1	C	470	LEU	5.2
1	B	485	ILE	5.0
1	A	448	CYS	5.0
1	D	694	ALA	5.0
1	B	486	GLU	4.9
1	B	630	ARG	4.9
1	C	471	VAL	4.8
1	B	470	LEU	4.8
1	A	446	GLU	4.8
1	C	486	GLU	4.7
1	B	471	VAL	4.7
1	A	470	LEU	4.6
1	A	694	ALA	4.6
1	C	674	TYR	4.5
1	B	469	GLN	4.4
1	D	481	LEU	4.4
1	D	772	VAL	4.4
1	C	627	ARG	4.3
1	D	627	ARG	4.3
1	D	524	GLY	4.2
1	D	516	ASP	4.2
1	A	699	ILE	4.1
1	B	694	ALA	4.1
1	C	741	ALA	4.1
1	B	693	PRO	4.1
1	C	772	VAL	4.0
1	A	467	ILE	4.0
1	D	695	ALA	4.0
1	C	694	ALA	4.0
1	A	777	CYS	3.9
1	B	749	TYR	3.9
1	D	523	MET	3.9
1	B	754	ALA	3.8
1	A	461	PHE	3.8
1	A	769	ALA	3.8
1	D	743	ALA	3.8
1	C	515	ARG	3.8
1	B	479	TYR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	746	ILE	3.8
1	A	698	TRP	3.8
1	C	467	ILE	3.8
1	B	777	CYS	3.8
1	D	828	LYS	3.8
1	C	628	PHE	3.7
1	D	699	ILE	3.7
1	C	476	ILE	3.7
1	D	482	GLU	3.7
1	C	773	GLY	3.6
1	A	744	GLY	3.6
1	C	769	ALA	3.6
1	C	523	MET	3.6
1	A	828	LYS	3.6
1	B	467	ILE	3.6
1	B	483	THR	3.6
1	A	466	GLU	3.5
1	A	778	ILE	3.5
1	C	695	ALA	3.5
1	B	772	VAL	3.5
1	B	698	TRP	3.5
1	B	741	ALA	3.5
1	D	745	SER	3.4
1	D	696	ILE	3.4
1	D	744	GLY	3.4
1	A	741	ALA	3.4
1	B	480	LYS	3.4
1	C	718	ARG	3.4
1	C	473	ALA	3.4
1	C	753	ALA	3.4
1	C	477	PRO	3.4
1	A	474	LYS	3.4
1	C	740	SER	3.4
1	A	479	TYR	3.4
1	B	487	THR	3.3
1	A	630	ARG	3.3
1	C	743	ALA	3.3
1	B	620	GLU	3.3
1	D	747	GLY	3.3
1	C	487	THR	3.3
1	C	757	VAL	3.3
1	B	756	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	695	ALA	3.3
1	B	757	VAL	3.3
1	A	773	GLY	3.3
1	A	462	LEU	3.3
1	C	749	TYR	3.2
1	A	481	LEU	3.2
1	A	627	ARG	3.2
1	B	743	ALA	3.2
1	A	689	THR	3.2
1	D	693	PRO	3.2
1	A	748	GLY	3.2
1	C	745	SER	3.2
1	B	748	GLY	3.1
1	B	758	THR	3.1
1	C	698	TRP	3.1
1	A	693	PRO	3.1
1	B	523	MET	3.1
1	A	754	ALA	3.1
1	C	699	ILE	3.1
1	A	749	TYR	3.1
1	B	778	ILE	3.1
1	A	447	GLU	3.1
1	B	474	LYS	3.1
1	A	472	ASN	3.0
1	A	745	SER	3.0
1	C	742	MET	3.0
1	C	608	TRP	3.0
1	B	740	SER	3.0
1	D	490	ARG	2.9
1	B	473	ALA	2.9
1	C	524	GLY	2.9
1	A	829	ASP	2.9
1	A	443	ARG	2.9
1	D	487	THR	2.9
1	A	486	GLU	2.9
1	A	696	ILE	2.9
1	D	748	GLY	2.9
1	C	478	ALA	2.9
1	C	482	GLU	2.9
1	D	698	TRP	2.9
1	B	516	ASP	2.9
1	D	630	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	829	ASP	2.8
1	C	693	PRO	2.8
1	C	754	ALA	2.8
1	C	738	VAL	2.8
1	D	758	THR	2.8
1	D	511	TYR	2.8
1	C	829	ASP	2.8
1	D	778	ILE	2.8
1	C	747	GLY	2.8
1	B	828	LYS	2.8
1	A	760	ILE	2.8
1	C	744	GLY	2.8
1	B	613	GLU	2.8
1	D	777	CYS	2.8
1	A	771	ASN	2.7
1	C	548	GLU	2.7
1	C	490	ARG	2.7
1	A	672	HIS	2.7
1	A	798	PRO	2.7
1	D	749	TYR	2.7
1	A	695	ALA	2.7
1	B	753	ALA	2.7
1	D	753	ALA	2.7
1	B	737	LEU	2.7
1	D	786	PRO	2.7
1	A	524	GLY	2.7
1	A	743	ALA	2.7
1	A	740	SER	2.7
1	A	501	LYS	2.7
1	A	688	CYS	2.7
1	B	677	GLU	2.7
1	A	756	ILE	2.6
1	A	846	VAL	2.6
1	A	697	ASN	2.6
1	C	469	GLN	2.6
1	D	775	SER	2.6
1	D	773	GLY	2.6
1	C	719	GLU	2.6
1	D	737	LEU	2.6
1	D	515	ARG	2.6
1	C	771	ASN	2.6
1	A	444	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	494	ILE	2.6
1	B	674	TYR	2.6
1	C	464	ASP	2.6
1	A	758	THR	2.6
1	C	770	GLN	2.6
1	B	744	GLY	2.5
1	A	830	ASN	2.5
1	C	777	CYS	2.5
1	A	523	MET	2.5
1	C	616	ALA	2.5
1	C	670	LYS	2.5
1	B	745	SER	2.5
1	B	773	GLY	2.5
1	C	666	LYS	2.5
1	A	620	GLU	2.5
1	A	687	TYR	2.5
1	C	761	TYR	2.5
1	A	747	GLY	2.5
1	D	628	PHE	2.5
1	D	740	SER	2.5
1	B	846	VAL	2.5
1	C	768	ALA	2.4
1	B	769	ALA	2.4
1	C	775	SER	2.4
1	B	628	PHE	2.4
1	B	738	VAL	2.4
1	C	488	HIS	2.4
1	A	575	LEU	2.4
1	C	480	LYS	2.4
1	B	696	ILE	2.4
1	B	488	HIS	2.4
1	B	751	ALA	2.4
1	B	688	CYS	2.4
1	B	719	GLU	2.3
1	B	750	ASN	2.3
1	C	481	LEU	2.3
1	C	617	VAL	2.3
1	B	673	GLU	2.3
1	C	748	GLY	2.3
1	D	787	THR	2.3
1	B	671	LEU	2.3
1	C	571	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	761	TYR	2.3
1	C	494	ILE	2.3
1	A	624	SER	2.2
1	A	751	ALA	2.2
1	B	747	GLY	2.2
1	D	769	ALA	2.2
1	B	608	TRP	2.2
1	A	774	SER	2.2
1	B	633	LYS	2.2
1	A	768	ALA	2.2
1	B	776	ASN	2.2
1	B	666	LYS	2.2
1	A	739	GLY	2.2
1	B	739	GLY	2.2
1	D	738	VAL	2.2
1	C	516	ASP	2.2
1	C	620	GLU	2.2
1	B	752	HIS	2.2
1	C	860	GLY	2.2
1	A	692	LYS	2.2
1	D	497	GLN	2.1
1	C	780	LEU	2.1
1	D	774	SER	2.1
1	A	445	ASN	2.1
1	B	771	ASN	2.1
1	D	754	ALA	2.1
1	A	490	ARG	2.1
1	B	597	PRO	2.1
1	C	630	ARG	2.1
1	D	510	GLN	2.1
1	C	613	GLU	2.1
1	D	620	GLU	2.1
1	D	776	ASN	2.1
1	A	738	VAL	2.1
1	B	501	LYS	2.1
1	C	828	LYS	2.1
1	B	472	ASN	2.1
1	A	789	GLU	2.1
1	A	628	PHE	2.1
1	B	524	GLY	2.1
1	A	775	SER	2.1
1	D	741	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	775	SER	2.1
1	C	723	THR	2.0
1	B	482	GLU	2.0
1	A	515	ARG	2.0
1	A	674	TYR	2.0
1	D	842	VAL	2.0
1	D	771	ASN	2.0
1	D	756	ILE	2.0
1	D	757	VAL	2.0
1	A	545	CYS	2.0
1	C	466	GLU	2.0
1	C	739	GLY	2.0
1	C	789	GLU	2.0
1	A	799	SER	2.0
1	C	800	ILE	2.0
1	D	742	MET	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(Å 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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.