Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 05:19 PM EDT

PDB ID	:	3RHP
Title	:	Crystal structure of the C707A mutant of the C-Terminal domain of 10'FOR MYLTETRAHYDROFOLATE DEHYDROGENASE
Authors	:	Tsybovsky, Y.
Deposited on	:	2011-04-11
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

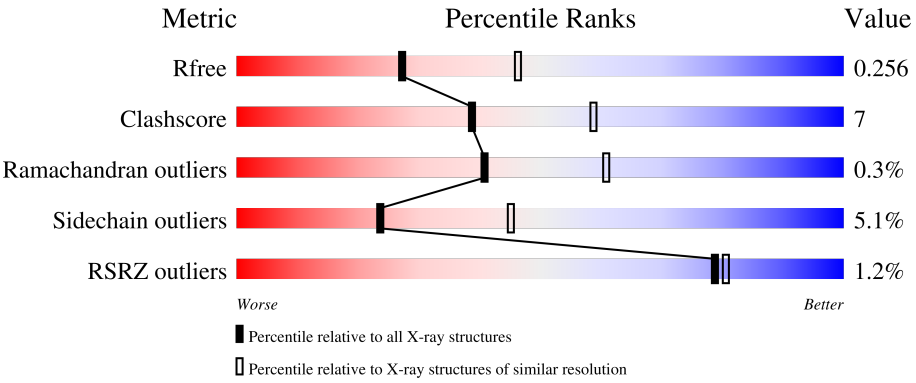
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	517	2% 75% 19%
1	B	517	76% 19%
1	C	517	77% 18%
1	D	517	77% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	3	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16351 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 Aldehyde dehydrogenase 1 family, member L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total 3867	C 2461	N 659	O 727	S 20	0	12	0
1	B	498	Total 3871	C 2461	N 664	O 726	S 20	0	11	0
1	C	498	Total 3866	C 2457	N 669	O 720	S 20	0	11	0
1	D	498	Total 3889	C 2473	N 667	O 729	S 20	0	13	0

There are 48 discrepancies between the modelled and reference sequences:

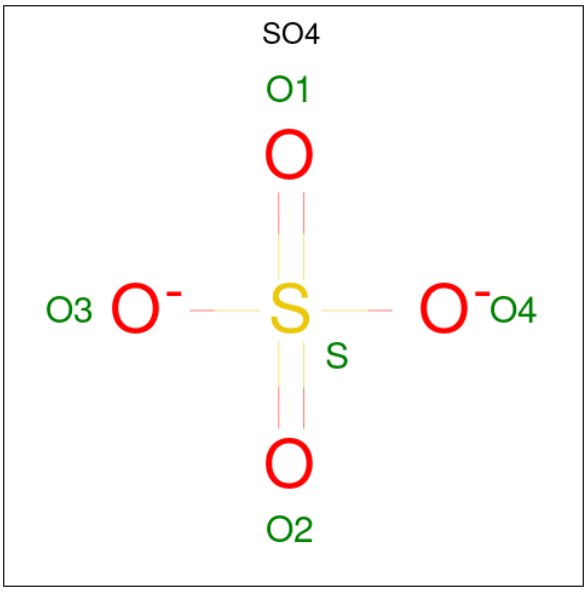
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HZB2
A	387	ARG	-	expression tag	UNP Q5HZB2
A	388	GLY	-	expression tag	UNP Q5HZB2
A	389	SER	-	expression tag	UNP Q5HZB2
A	390	HIS	-	expression tag	UNP Q5HZB2
A	391	HIS	-	expression tag	UNP Q5HZB2
A	392	HIS	-	expression tag	UNP Q5HZB2
A	393	HIS	-	expression tag	UNP Q5HZB2
A	394	HIS	-	expression tag	UNP Q5HZB2
A	395	THR	-	expression tag	UNP Q5HZB2
A	396	THR	-	expression tag	UNP Q5HZB2
A	707	ALA	CYS	engineered mutation	UNP Q5HZB2
B	386	MET	-	expression tag	UNP Q5HZB2
B	387	ARG	-	expression tag	UNP Q5HZB2
B	388	GLY	-	expression tag	UNP Q5HZB2
B	389	SER	-	expression tag	UNP Q5HZB2
B	390	HIS	-	expression tag	UNP Q5HZB2
B	391	HIS	-	expression tag	UNP Q5HZB2
B	392	HIS	-	expression tag	UNP Q5HZB2
B	393	HIS	-	expression tag	UNP Q5HZB2
B	394	HIS	-	expression tag	UNP Q5HZB2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HZB2
B	396	THR	-	expression tag	UNP Q5HZB2
B	707	ALA	CYS	engineered mutation	UNP Q5HZB2
C	386	MET	-	expression tag	UNP Q5HZB2
C	387	ARG	-	expression tag	UNP Q5HZB2
C	388	GLY	-	expression tag	UNP Q5HZB2
C	389	SER	-	expression tag	UNP Q5HZB2
C	390	HIS	-	expression tag	UNP Q5HZB2
C	391	HIS	-	expression tag	UNP Q5HZB2
C	392	HIS	-	expression tag	UNP Q5HZB2
C	393	HIS	-	expression tag	UNP Q5HZB2
C	394	HIS	-	expression tag	UNP Q5HZB2
C	395	THR	-	expression tag	UNP Q5HZB2
C	396	THR	-	expression tag	UNP Q5HZB2
C	707	ALA	CYS	engineered mutation	UNP Q5HZB2
D	386	MET	-	expression tag	UNP Q5HZB2
D	387	ARG	-	expression tag	UNP Q5HZB2
D	388	GLY	-	expression tag	UNP Q5HZB2
D	389	SER	-	expression tag	UNP Q5HZB2
D	390	HIS	-	expression tag	UNP Q5HZB2
D	391	HIS	-	expression tag	UNP Q5HZB2
D	392	HIS	-	expression tag	UNP Q5HZB2
D	393	HIS	-	expression tag	UNP Q5HZB2
D	394	HIS	-	expression tag	UNP Q5HZB2
D	395	THR	-	expression tag	UNP Q5HZB2
D	396	THR	-	expression tag	UNP Q5HZB2
D	707	ALA	CYS	engineered mutation	UNP Q5HZB2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



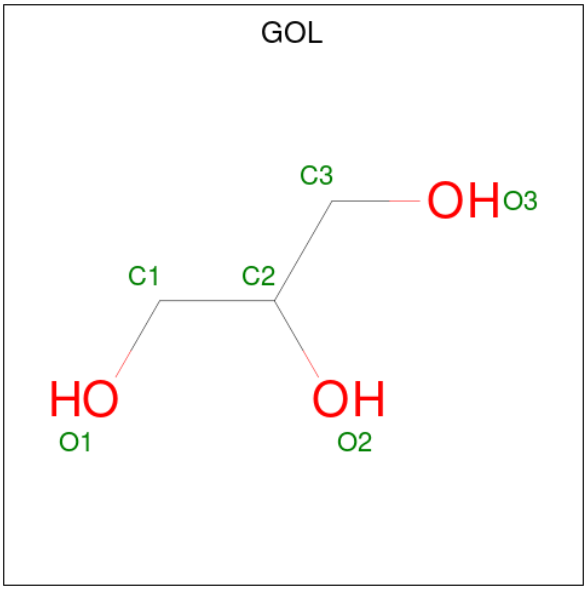
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

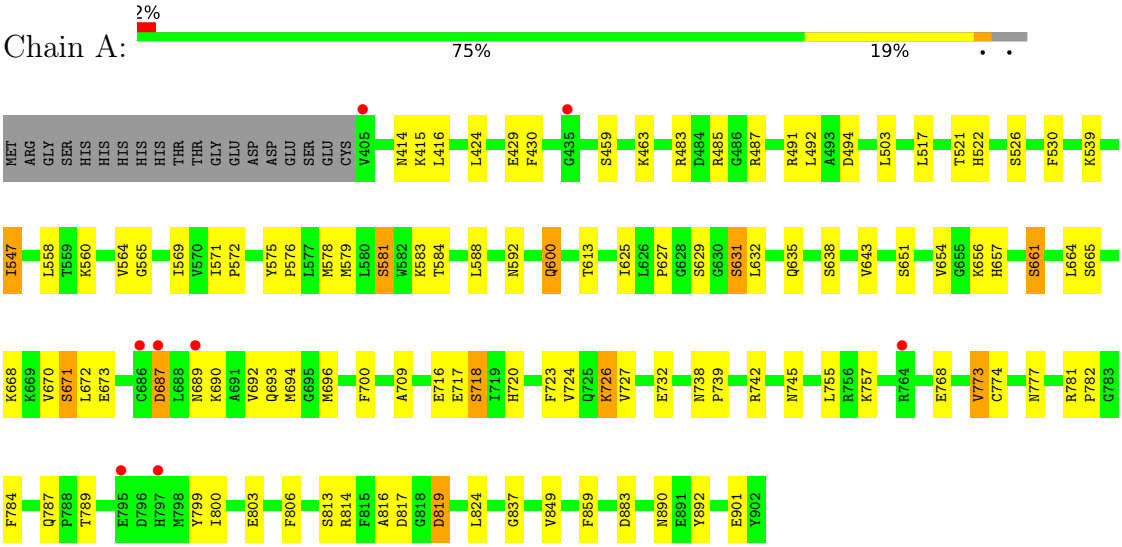
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	176	Total O 176 176	0	0
4	B	170	Total O 170 170	0	0
4	C	185	Total O 185 185	0	0
4	D	183	Total O 183 183	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

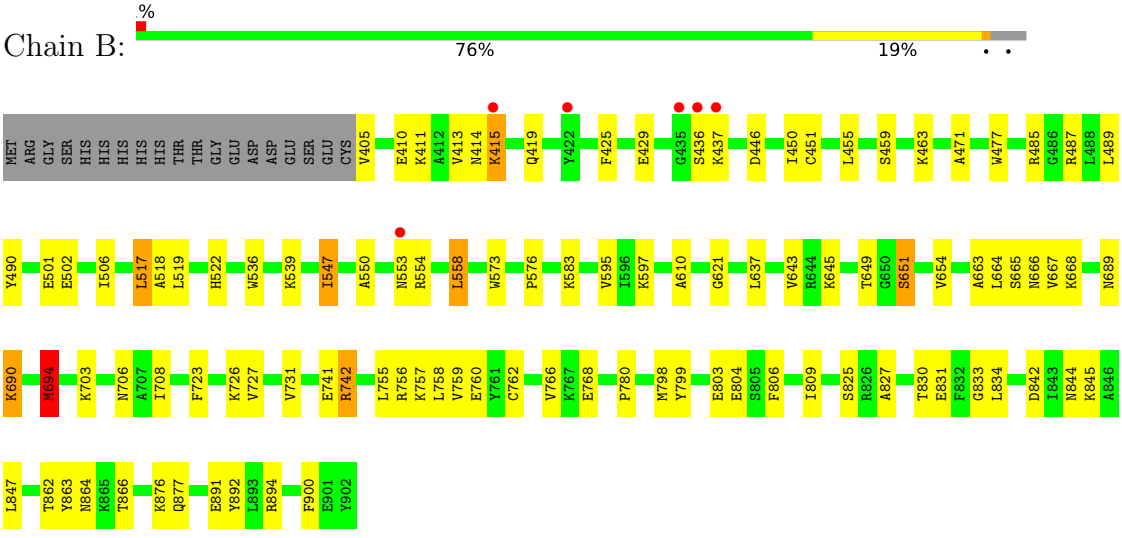
• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

Chain A:



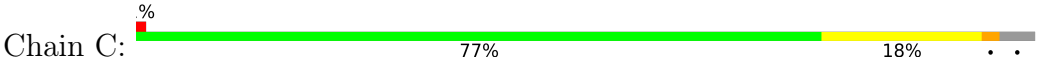
• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

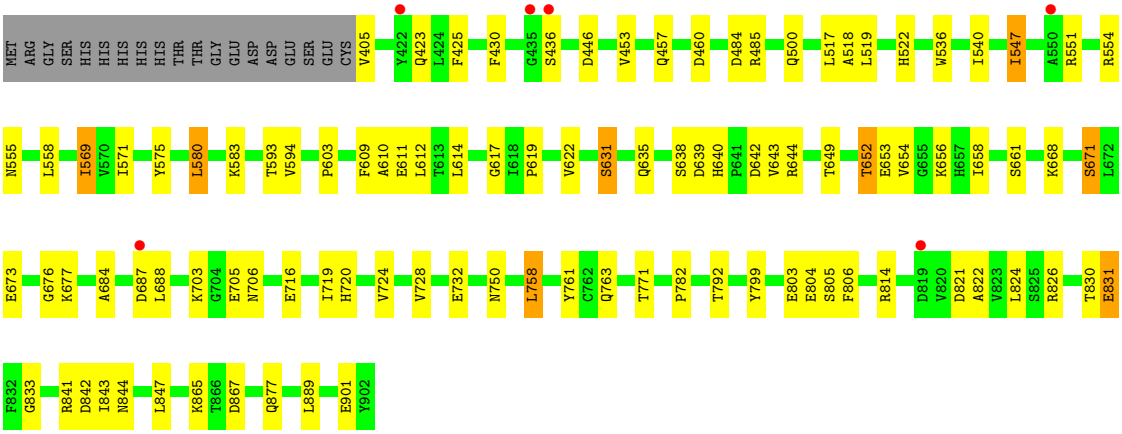
Chain B:



• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

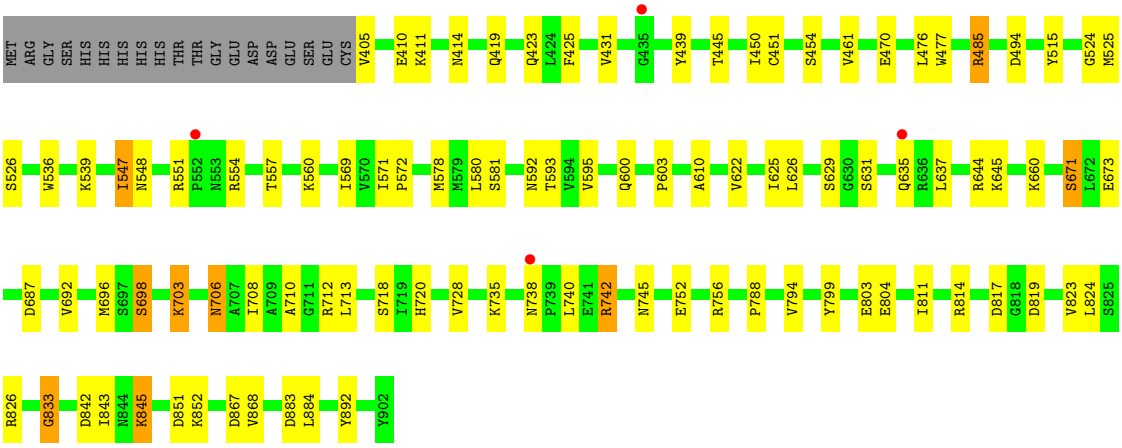
Chain C:





• Molecule 1: Aldehyde dehydrogenase 1 family, member L1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.40Å 194.90Å 97.11Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	48.97 – 2.50 48.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.97-2.50) 98.0 (48.94-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.257 0.214 , 0.256	Depositor DCC
R_{free} test set	7861 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16351	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	1.07	4/3985 (0.1%)	1.00	4/5394 (0.1%)
1	B	1.04	1/3993 (0.0%)	0.98	6/5403 (0.1%)
1	C	1.14	2/3991 (0.1%)	1.05	8/5400 (0.1%)
1	D	1.08	3/4015 (0.1%)	1.01	8/5430 (0.1%)
All	All	1.08	10/15984 (0.1%)	1.01	26/21627 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	742	ARG	CG-CD	6.56	1.68	1.51
1	C	831	GLU	CG-CD	6.39	1.61	1.51
1	B	827	ALA	CA-CB	-6.36	1.39	1.52
1	D	738	ASN	CB-CG	6.30	1.65	1.51
1	A	491	ARG	CB-CG	5.70	1.68	1.52
1	D	515	TYR	CD1-CE1	5.52	1.47	1.39
1	A	709	ALA	CA-CB	-5.32	1.41	1.52
1	A	890	ASN	CB-CG	5.20	1.63	1.51
1	C	653	GLU	CB-CG	5.12	1.61	1.52
1	A	716	GLU	CG-CD	5.08	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	485	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	D	826	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	C	484	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	687	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	503	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	D	644	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	485	ARG	NE-CZ-NH2	-6.34	117.13	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	446	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	687	ASP	CB-CG-OD2	6.12	123.81	118.30
1	B	894	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	B	517	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	687	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	485	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	519	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	487	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	694[A]	MET	CG-SD-CE	5.54	109.07	100.20
1	B	694[B]	MET	CG-SD-CE	5.54	109.07	100.20
1	D	494	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	842	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	758	LEU	CA-CB-CG	-5.30	103.11	115.30
1	D	551	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	575	TYR	CA-CB-CG	5.25	123.38	113.40
1	D	712	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	851	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	C	639	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	494	ASP	CB-CG-OD2	5.04	122.84	118.30

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	3867	0	3861	59	0
1	B	3871	0	3869	69	0
1	C	3866	0	3867	61	0
1	D	3889	0	3898	57	0
2	A	30	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	2	0
2	D	20	0	0	1	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	176	0	0	2	0
4	B	170	0	0	6	0
4	C	185	0	0	7	0
4	D	183	0	0	8	0
All	All	16351	0	15527	234	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 7.

All (234) 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:B:690:LYS:HE3	1:B:694[B]:MET:CE	1.29	1.56
1:B:690:LYS:CE	1:B:694[B]:MET:CE	1.99	1.37
1:B:690:LYS:CE	1:B:694[B]:MET:HE1	1.72	1.12
1:B:690:LYS:HE3	1:B:694[B]:MET:SD	1.94	1.06
1:D:756:ARG:NH2	4:D:1159:HOH:O	1.88	1.04
1:B:690:LYS:HE3	1:B:694[B]:MET:HE3	1.06	1.03
1:B:690:LYS:CE	1:B:694[B]:MET:HE3	1.76	1.02
1:B:690:LYS:NZ	1:B:694[B]:MET:CE	2.37	0.86
1:B:690:LYS:NZ	1:B:694[B]:MET:HE1	1.90	0.85
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:HH11	1.42	0.82
1:B:410:GLU:OE1	1:B:419[B]:GLN:NE2	2.11	0.82
1:A:773:VAL:O	1:A:774:CYS:HB3	1.81	0.78
1:B:799:TYR:CE2	1:B:803[B]:GLU:HG3	2.18	0.78
1:B:414:ASN:O	1:B:415:LYS:HB2	1.84	0.76
1:B:727:VAL:O	1:B:731:VAL:HG23	1.87	0.75
1:C:684:ALA:HA	1:C:719:ILE:HD13	1.69	0.75
1:D:756:ARG:NE	4:D:1161:HOH:O	2.23	0.70
1:C:500:GLN:OE1	4:C:1093:HOH:O	2.08	0.70
1:C:457:GLN:O	1:C:460:ASP:HB2	1.92	0.69
1:A:547:ILE:HD13	1:A:547:ILE:H	1.57	0.69
1:A:720:HIS:CD2	1:A:814:ARG:HG3	2.27	0.69
1:C:593:THR:HG22	1:C:622:VAL:HG13	1.75	0.68
1:A:459:SER:O	1:A:463:LYS:HG3	1.94	0.68
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.28	0.67
1:B:780:PRO:O	4:B:1071:HOH:O	2.12	0.67
1:D:423:GLN:HA	1:D:454:SER:OG	1.95	0.66
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:LYS:NZ	1:B:694[B]:MET:HE3	2.07	0.65
1:D:718:SER:HB3	1:D:817:ASP:OD1	1.97	0.65
1:B:690:LYS:HE2	1:B:694[B]:MET:HE1	1.74	0.65
1:B:844:ASN:ND2	1:C:841[B]:ARG:HH12	1.95	0.65
1:D:631:SER:O	1:D:635:GLN:HB2	1.98	0.64
1:B:689:ASN:OD1	1:B:726:LYS:NZ	2.29	0.64
1:D:842:ASP:HB3	1:D:845:LYS:HB2	1.79	0.64
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:NH1	2.09	0.64
1:C:551:ARG:NH2	2:C:3:SO4:O4	2.31	0.63
1:B:690:LYS:CE	1:B:694[B]:MET:SD	2.72	0.62
1:C:518:ALA:HA	1:C:522:HIS:HB2	1.83	0.61
1:B:539:LYS:HD3	1:D:536:TRP:CE2	2.37	0.59
1:B:558:LEU:HD12	1:B:558:LEU:C	2.23	0.59
1:D:868:VAL:HG13	4:D:1017:HOH:O	2.03	0.58
1:D:600:GLN:NE2	1:D:629:SER:HA	2.18	0.58
1:A:569:ILE:HD12	1:A:571:ILE:HD11	1.86	0.58
1:D:526:SER:OG	1:D:578:MET:HA	2.03	0.58
1:A:558:LEU:C	1:A:558:LEU:HD12	2.23	0.58
1:A:777:ASN:O	1:A:787:GLN:HG3	2.04	0.58
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.85	0.58
1:B:690:LYS:HZ1	1:B:694[B]:MET:HE1	1.68	0.57
1:C:831:GLU:HB2	4:C:1119:HOH:O	2.03	0.57
1:A:564:VAL:HG23	1:A:565:GLY:N	2.19	0.57
1:A:692:VAL:HG21	1:A:726:LYS:HB3	1.87	0.57
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.40	0.57
1:D:804:GLU:HA	4:D:1046:HOH:O	2.03	0.57
1:C:540:ILE:HD11	1:C:889:LEU:HD22	1.87	0.56
1:A:651:SER:OG	1:A:654:VAL:HG23	2.06	0.56
1:B:762:CYS:O	1:B:766:VAL:HG23	2.05	0.56
1:D:470:GLU:HG3	4:D:1032:HOH:O	2.06	0.56
1:B:536:TRP:CE2	1:D:539:LYS:HD3	2.41	0.56
1:C:643:VAL:O	1:C:668:LYS:HE3	2.06	0.56
1:C:671:SER:HB2	4:C:1098:HOH:O	2.05	0.55
1:A:720:HIS:O	1:A:724:VAL:HG23	2.07	0.55
1:A:781[B]:ARG:HB2	1:A:782:PRO:HD2	1.88	0.55
1:C:640:HIS:CE1	1:C:642:ASP:HB2	2.42	0.55
1:A:671:SER:O	1:A:672:LEU:HD23	2.06	0.55
1:A:517:LEU:HD23	1:A:521:THR:HB	1.89	0.55
1:D:445:THR:O	1:D:445:THR:HG22	2.06	0.55
1:C:684:ALA:N	1:C:716:GLU:OE2	2.32	0.55
1:A:539:LYS:HD3	1:C:536:TRP:CE2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:GLY:HA2	1:A:859:PHE:O	2.08	0.54
1:A:414:ASN:O	1:A:415:LYS:HB2	2.06	0.54
1:A:781[B]:ARG:HB2	1:A:782:PRO:CD	2.37	0.54
1:B:643:VAL:O	1:B:668:LYS:HE3	2.07	0.54
1:D:883:ASP:O	1:D:884:LEU:HB2	2.08	0.54
1:C:569:ILE:HG13	1:C:571:ILE:HD11	1.91	0.53
1:A:718:SER:HB3	1:A:817:ASP:OD1	2.09	0.53
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.44	0.53
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.44	0.52
1:D:592:ASN:ND2	1:D:892:TYR:HB3	2.24	0.52
1:D:692:VAL:O	1:D:696:MET:HG2	2.09	0.52
1:D:450:ILE:O	1:D:451:CYS:HB3	2.10	0.51
1:A:638:SER:HB3	1:A:661:SER:HB2	1.92	0.51
1:C:901:GLU:HG3	4:C:1040:HOH:O	2.11	0.51
1:D:811:ILE:O	1:D:811:ILE:HG22	2.09	0.51
1:C:547:ILE:HB	1:D:867:ASP:CG	2.30	0.51
1:D:580:LEU:C	1:D:580:LEU:HD23	2.31	0.51
1:C:676:GLY:O	1:C:804:GLU:HG3	2.11	0.51
1:C:554:ARG:NE	2:C:3:SO4:O1	2.35	0.51
1:D:560[A]:LYS:NZ	4:D:1170:HOH:O	2.44	0.51
1:A:424:LEU:O	1:A:430:PHE:HA	2.12	0.50
1:C:453:VAL:HG21	1:C:603:PRO:HG2	1.94	0.50
1:B:651:SER:OG	1:B:654:VAL:HG23	2.12	0.50
1:B:863:TYR:CD2	1:B:864:ASN:N	2.79	0.50
1:D:477:TRP:CH2	1:D:485:ARG:HG3	2.46	0.50
1:B:891:GLU:HB3	4:B:1056:HOH:O	2.10	0.50
1:D:698:SER:OG	1:D:710:ALA:HB3	2.12	0.50
1:C:558:LEU:C	1:C:558:LEU:HD12	2.32	0.50
1:C:654:VAL:O	1:C:658:ILE:HG12	2.12	0.50
1:B:758:LEU:HD22	1:B:809:ILE:HD11	1.94	0.49
1:B:708:ILE:HG22	1:B:834:LEU:HG	1.95	0.49
1:C:571:ILE:HD12	1:C:580:LEU:HA	1.94	0.49
1:D:425:PHE:CD2	1:D:610:ALA:HB1	2.47	0.49
1:A:521:THR:O	1:A:522:HIS:C	2.52	0.48
1:D:554:ARG:NE	2:D:2:SO4:O4	2.37	0.48
1:B:550:ALA:O	1:B:553:ASN:HB2	2.12	0.48
1:C:833:GLY:HA2	4:C:1013:HOH:O	2.14	0.48
1:C:644:ARG:HB3	4:C:1044:HOH:O	2.13	0.48
1:C:724:VAL:O	1:C:728:VAL:HG23	2.13	0.47
1:D:580:LEU:HD23	1:D:581:SER:N	2.30	0.47
1:A:656:LYS:HG2	1:B:663:ALA:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:HIS:CD2	1:D:814:ARG:HG3	2.49	0.47
1:B:842:ASP:C	1:B:842:ASP:OD2	2.53	0.47
1:A:547:ILE:H	1:A:547:ILE:CD1	2.27	0.47
1:C:758:LEU:HD23	1:C:758:LEU:HA	1.51	0.47
1:A:631:SER:O	1:A:632:LEU:C	2.51	0.46
1:C:425:PHE:CD2	1:C:610:ALA:HB1	2.50	0.46
1:A:583:LYS:HE2	1:A:883:ASP:OD2	2.15	0.46
1:A:687:ASP:OD2	4:A:1162:HOH:O	2.20	0.46
1:C:867:ASP:CG	1:D:547:ILE:HB	2.35	0.46
1:B:595:VAL:HG11	1:B:637:LEU:HD21	1.98	0.46
1:B:831:GLU:O	1:B:877:GLN:HB2	2.16	0.46
1:D:571:ILE:CG2	1:D:572:PRO:HD2	2.46	0.46
1:D:595:VAL:HG11	1:D:637:LEU:HD21	1.97	0.46
1:B:554:ARG:HH22	1:D:852:LYS:HE2	1.80	0.46
1:B:690:LYS:HE2	1:B:694[B]:MET:CE	2.28	0.46
1:A:816:ALA:HB3	1:A:819:ASP:HB2	1.98	0.46
1:B:554:ARG:NH2	1:D:852:LYS:HE2	2.30	0.46
1:C:617:GLY:O	1:C:619:PRO:HD3	2.16	0.46
1:A:781[A]:ARG:HB2	1:A:782:PRO:CD	2.45	0.46
1:B:583:LYS:HE3	1:B:649:THR:OG1	2.16	0.46
1:C:547:ILE:HD11	1:C:555:ASN:HB3	1.98	0.46
1:A:690:LYS:HE3	1:A:694[B]:MET:HE1	1.96	0.45
1:A:693:GLN:HA	1:A:693:GLN:OE1	2.16	0.45
1:A:781[A]:ARG:HB2	1:A:782:PRO:HD2	1.98	0.45
1:D:706:ASN:ND2	1:D:708:ILE:H	2.13	0.45
1:A:592:ASN:HD21	1:A:892:TYR:HB3	1.81	0.45
1:D:593:THR:HG22	1:D:622:VAL:HA	1.99	0.45
1:B:450:ILE:O	1:B:451:CYS:HB3	2.16	0.45
1:A:600:GLN:NE2	1:A:629:SER:HA	2.31	0.44
1:B:411:LYS:HD3	4:B:1154:HOH:O	2.17	0.44
1:B:690:LYS:HZ2	1:B:694[B]:MET:HE3	1.77	0.44
1:B:833:GLY:HA2	4:B:1027:HOH:O	2.18	0.44
1:C:720:HIS:O	1:C:724:VAL:HG23	2.16	0.44
1:D:439:TYR:OH	1:D:603:PRO:HG3	2.18	0.44
1:D:706:ASN:C	1:D:706:ASN:HD22	2.20	0.44
1:A:901:GLU:HB3	1:B:862:THR:HB	1.98	0.44
1:B:866:THR:OG1	3:B:10:GOL:H11	2.17	0.44
1:A:530:PHE:CE1	1:A:581:SER:HB3	2.52	0.44
1:D:547:ILE:HD12	1:D:557:THR:OG1	2.18	0.44
1:B:755:LEU:O	1:B:759:VAL:HG23	2.18	0.44
1:B:803[A]:GLU:HG3	1:B:804:GLU:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:LEU:HD12	1:C:688:LEU:HA	1.75	0.44
1:D:425:PHE:CG	1:D:610:ALA:HB1	2.53	0.44
1:A:774:CYS:O	1:A:789:THR:HA	2.17	0.44
1:C:631:SER:O	1:C:635:GLN:HB3	2.18	0.44
1:A:696:MET:HE3	1:A:700:PHE:CE2	2.52	0.43
1:B:501:GLU:HB2	4:B:1017:HOH:O	2.18	0.43
1:A:643:VAL:O	1:A:668:LYS:HE3	2.18	0.43
1:D:571:ILE:HG23	1:D:572:PRO:HD2	2.00	0.43
1:D:713:LEU:HD12	1:D:713:LEU:N	2.33	0.43
1:A:689:ASN:OD1	1:A:726:LYS:NZ	2.51	0.43
1:C:705:GLU:OE1	1:C:750:ASN:HB2	2.18	0.43
1:C:831:GLU:HB3	1:C:877:GLN:HG3	2.01	0.43
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.84	0.43
1:C:638:SER:HB3	1:C:661:SER:HB2	2.00	0.43
1:C:865:LYS:O	1:C:865:LYS:HG3	2.18	0.43
1:D:410:GLU:HG3	1:D:419[B]:GLN:NE2	2.34	0.43
1:C:583:LYS:HE2	1:C:649:THR:OG1	2.19	0.43
1:D:414:ASN:HB2	1:D:740:LEU:HD22	2.00	0.43
1:A:592:ASN:ND2	1:A:892:TYR:HB3	2.34	0.43
1:C:843:ILE:HG23	1:C:844:ASN:N	2.33	0.43
1:C:847:LEU:HD23	1:C:847:LEU:HA	1.76	0.43
1:A:635:GLN:OE1	1:A:657[A]:HIS:NE2	2.50	0.42
1:A:768[B]:GLU:OE2	1:A:800:ILE:HG12	2.19	0.42
1:D:671:SER:HB2	4:D:1092:HOH:O	2.18	0.42
1:B:547:ILE:HD13	1:B:547:ILE:H	1.84	0.42
1:B:876:LYS:HE2	4:B:1008:HOH:O	2.20	0.42
1:D:423:GLN:HB3	1:D:431:VAL:O	2.19	0.42
1:B:471:ALA:HB2	1:B:621:GLY:HA3	2.00	0.42
1:B:573:TRP:O	1:B:576:PRO:HD3	2.18	0.42
1:B:666:ASN:O	1:B:667:VAL:CG2	2.67	0.42
1:C:423:GLN:HB2	1:C:430:PHE:HB3	2.00	0.42
1:B:645:LYS:HE3	1:B:892:TYR:CE1	2.54	0.42
1:C:609:PHE:O	1:C:612:LEU:HB2	2.19	0.42
1:C:706:ASN:HD21	3:C:8:GOL:H31	1.84	0.42
1:D:571:ILE:HD12	1:D:580:LEU:HA	2.02	0.42
1:A:572:PRO:HG2	1:A:579:MET:HG3	2.02	0.42
1:A:632:LEU:C	1:A:632:LEU:HD23	2.40	0.42
1:C:569:ILE:HD13	1:C:594:VAL:HG21	2.00	0.42
1:D:833:GLY:HA2	4:D:1022:HOH:O	2.20	0.42
1:B:723:PHE:O	1:B:727:VAL:HG23	2.20	0.42
1:C:720:HIS:CD2	1:C:814:ARG:HG3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:LYS:HE3	1:B:760:GLU:OE1	2.20	0.42
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.75	0.42
1:A:575:TYR:O	1:A:576:PRO:C	2.58	0.41
1:C:821:ASP:HA	1:C:824:LEU:HD12	2.02	0.41
1:A:738:ASN:OD1	1:A:739:PRO:HD2	2.19	0.41
1:B:459:SER:O	1:B:463:LYS:HG3	2.20	0.41
1:B:477:TRP:CH2	1:B:485:ARG:HG3	2.55	0.41
1:B:768[B]:GLU:HG3	1:B:798:MET:HG2	2.02	0.41
1:C:536:TRP:CG	1:C:889:LEU:HD11	2.55	0.41
1:D:823:VAL:HG13	1:D:824:LEU:N	2.35	0.41
1:A:424:LEU:CD2	1:A:627:PRO:HD2	2.51	0.41
1:A:782:PRO:HG2	4:A:1109:HOH:O	2.20	0.41
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.83	0.41
1:B:425:PHE:CD2	1:B:610:ALA:HB1	2.55	0.41
1:C:831:GLU:OE1	1:C:877:GLN:HG3	2.20	0.41
1:D:752:GLU:HG2	1:D:756:ARG:HH21	1.84	0.41
1:A:664:LEU:HD23	1:A:664:LEU:HA	1.86	0.41
1:B:518:ALA:HA	1:B:522:HIS:HB2	2.01	0.41
1:C:677:LYS:HA	4:C:1097:HOH:O	2.20	0.41
1:D:706:ASN:ND2	1:D:706:ASN:C	2.74	0.41
1:A:755:LEU:HD22	1:A:784:PHE:HB3	2.02	0.41
1:B:799:TYR:CD2	1:B:803[B]:GLU:HG3	2.55	0.41
1:C:611:GLU:O	1:C:614:LEU:HB2	2.20	0.41
1:C:822:ALA:O	1:C:826:ARG:HG3	2.21	0.41
1:D:571:ILE:CD1	1:D:580:LEU:HA	2.51	0.41
1:A:492:LEU:HD13	1:A:613:THR:HA	2.03	0.41
1:B:547:ILE:HD13	1:B:547:ILE:N	2.36	0.40
1:B:490[A]:TYR:O	1:B:490[A]:TYR:CD2	2.73	0.40
1:C:652:THR:HG22	1:C:656:LYS:HE3	2.04	0.40
1:A:526:SER:OG	1:A:578:MET:HA	2.21	0.40
1:A:584:THR:HG22	1:A:588:LEU:HG	2.03	0.40
1:B:446:ASP:C	1:B:446:ASP:OD2	2.60	0.40
1:B:502:GLU:O	1:B:506:ILE:HG13	2.21	0.40
1:B:900:PHE:HD2	1:D:843:ILE:HD11	1.86	0.40
1:D:461:VAL:HA	1:D:626:LEU:HD11	2.03	0.40
1:A:723:PHE:O	1:A:727:VAL:HG23	2.22	0.40
1:C:761:TYR:CZ	1:C:805:SER:HB3	2.56	0.40
1:D:569:ILE:HD13	1:D:569:ILE:HG21	1.88	0.40
1:A:670:VAL:HG22	1:A:671:SER:N	2.35	0.40
1:C:771:THR:HB	1:C:792:THR:OG1	2.22	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	507/517 (98%)	484 (96%)	23 (4%)	0	100	100
1	B	507/517 (98%)	477 (94%)	29 (6%)	1 (0%)	47	68
1	C	507/517 (98%)	479 (94%)	27 (5%)	1 (0%)	47	68
1	D	509/517 (98%)	470 (92%)	36 (7%)	3 (1%)	25	43
All	All	2030/2068 (98%)	1910 (94%)	115 (6%)	5 (0%)	41	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	436	SER
1	D	524	GLY
1	B	436	SER
1	D	703	LYS
1	D	833	GLY

5.3.2 Protein sidechains (i)

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	415/425 (98%)	391 (94%)	24 (6%)	20	38
1	B	416/425 (98%)	390 (94%)	26 (6%)	18	34
1	C	415/425 (98%)	401 (97%)	14 (3%)	37	63
1	D	419/425 (99%)	399 (95%)	20 (5%)	25	48
All	All	1665/1700 (98%)	1581 (95%)	84 (5%)	24	46

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LEU
1	A	429	GLU
1	A	487	ARG
1	A	547	ILE
1	A	560	LYS
1	A	581	SER
1	A	600	GLN
1	A	625	ILE
1	A	631	SER
1	A	661	SER
1	A	665	SER
1	A	671	SER
1	A	673	GLU
1	A	717	GLU
1	A	718	SER
1	A	726	LYS
1	A	732	GLU
1	A	742	ARG
1	A	745	ASN
1	A	757	LYS
1	A	773	VAL
1	A	806	PHE
1	A	813	SER
1	A	819	ASP
1	B	405	VAL
1	B	413	VAL
1	B	415	LYS
1	B	429	GLU
1	B	437	LYS
1	B	455	LEU
1	B	517	LEU
1	B	547	ILE
1	B	558	LEU
1	B	597	LYS
1	B	651	SER
1	B	664	LEU
1	B	665	SER
1	B	690	LYS
1	B	694[A]	MET
1	B	694[B]	MET
1	B	703	LYS
1	B	706	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	741[A]	GLU
1	B	741[B]	GLU
1	B	742	ARG
1	B	756	ARG
1	B	806	PHE
1	B	825	SER
1	B	830	THR
1	B	845	LYS
1	C	405	VAL
1	C	517	LEU
1	C	519	LEU
1	C	547	ILE
1	C	569	ILE
1	C	580	LEU
1	C	631	SER
1	C	652	THR
1	C	671	SER
1	C	673	GLU
1	C	703	LYS
1	C	732	GLU
1	C	806	PHE
1	C	830	THR
1	D	405	VAL
1	D	411	LYS
1	D	476	LEU
1	D	525	MET
1	D	547	ILE
1	D	625	ILE
1	D	645	LYS
1	D	660	LYS
1	D	671	SER
1	D	673	GLU
1	D	698	SER
1	D	703	LYS
1	D	706	ASN
1	D	728	VAL
1	D	735	LYS
1	D	742	ARG
1	D	745	ASN
1	D	788	PRO
1	D	819	ASP
1	D	845	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	600	GLN
1	A	706	ASN
1	A	745	ASN
1	A	750	ASN
1	B	541	GLN
1	B	600	GLN
1	B	706	ASN
1	B	745	ASN
1	B	844	ASN
1	C	541	GLN
1	C	600	GLN
1	C	706	ASN
1	C	750	ASN
1	D	474	ASN
1	D	548	ASN
1	D	600	GLN
1	D	706	ASN
1	D	745	ASN
1	D	750	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 monosaccharides in this entry.

5.6 Ligand geometry

28 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	$\#\|Z\| > 2$
3	GOL	A	7	-	5,5,5	0.33	0	5,5,5	1.45	1 (20%)
2	SO4	C	6	-	4,4,4	0.19	0	6,6,6	1.10	0
2	SO4	A	3	-	4,4,4	0.40	0	6,6,6	0.69	0
2	SO4	C	4	-	4,4,4	0.28	0	6,6,6	0.60	0
2	SO4	D	2	-	4,4,4	0.46	0	6,6,6	0.59	0
3	GOL	C	8	-	5,5,5	0.62	0	5,5,5	2.07	2 (40%)
2	SO4	B	4	-	4,4,4	0.16	0	6,6,6	0.56	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.80	0
2	SO4	D	1	-	4,4,4	0.33	0	6,6,6	0.58	0
2	SO4	C	5	-	4,4,4	0.09	0	6,6,6	0.65	0
2	SO4	B	3	-	4,4,4	0.21	0	6,6,6	0.59	0
2	SO4	A	4	-	4,4,4	0.20	0	6,6,6	0.88	0
3	GOL	D	5	-	5,5,5	0.65	0	5,5,5	1.15	0
2	SO4	D	4	-	4,4,4	0.14	0	6,6,6	0.57	0
2	SO4	C	7	-	4,4,4	0.41	0	6,6,6	0.78	0
2	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.59	0
2	SO4	D	3	-	4,4,4	0.18	0	6,6,6	0.79	0
2	SO4	C	3	-	4,4,4	0.13	0	6,6,6	0.45	0
2	SO4	B	6	-	4,4,4	0.23	0	6,6,6	0.52	0
2	SO4	B	5	-	4,4,4	0.33	0	6,6,6	0.67	0
2	SO4	B	8	-	4,4,4	0.21	0	6,6,6	0.60	0
2	SO4	B	7	-	4,4,4	0.09	0	6,6,6	0.85	0
2	SO4	B	9	-	4,4,4	0.27	0	6,6,6	0.63	0
2	SO4	A	2	-	4,4,4	0.33	0	6,6,6	0.80	0
3	GOL	B	10	-	5,5,5	0.37	0	5,5,5	1.87	1 (20%)
2	SO4	A	6	-	4,4,4	0.22	0	6,6,6	1.51	1 (16%)
2	SO4	C	2	-	4,4,4	0.20	0	6,6,6	0.62	0
2	SO4	A	5	-	4,4,4	0.42	0	6,6,6	1.41	0

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
3	GOL	A	7	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	10	-	-	2/4/4/4	-
3	GOL	D	5	-	-	2/4/4/4	-
3	GOL	C	8	-	-	3/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	10	GOL	C3-C2-C1	-3.80	96.95	111.70
3	C	8	GOL	C3-C2-C1	-3.39	98.51	111.70
3	A	7	GOL	C3-C2-C1	-2.95	100.25	111.70
2	A	6	SO4	O4-S-O3	2.80	121.02	109.06
3	C	8	GOL	O2-C2-C3	2.01	118.00	109.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	7	GOL	C1-C2-C3-O3
3	B	10	GOL	C1-C2-C3-O3
3	C	8	GOL	C1-C2-C3-O3
3	D	5	GOL	O1-C1-C2-C3
3	D	5	GOL	O1-C1-C2-O2
3	A	7	GOL	O2-C2-C3-O3
3	B	10	GOL	O2-C2-C3-O3
3	C	8	GOL	O2-C2-C3-O3
3	C	8	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	SO4	1	0
3	C	8	GOL	1	0
2	C	3	SO4	2	0
3	B	10	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	498/517 (96%)	-0.07	8 (1%)	72	74	16, 31, 46, 57	19 (3%)
1	B	498/517 (96%)	-0.06	6 (1%)	79	80	19, 32, 46, 62	20 (4%)
1	C	498/517 (96%)	-0.23	6 (1%)	79	80	15, 28, 39, 53	16 (3%)
1	D	498/517 (96%)	-0.21	4 (0%)	86	87	16, 31, 44, 62	19 (3%)
All	All	1992/2068 (96%)	-0.15	24 (1%)	79	80	15, 30, 44, 62	74 (3%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	435	GLY	3.2
1	B	436	SER	3.0
1	D	738	ASN	2.8
1	A	764	ARG	2.7
1	B	553	ASN	2.6
1	A	405	VAL	2.6
1	A	435	GLY	2.6
1	B	415	LYS	2.6
1	C	422	TYR	2.5
1	C	687	ASP	2.5
1	B	422	TYR	2.4
1	D	552	PRO	2.3
1	A	797	HIS	2.3
1	A	795[A]	GLU	2.2
1	C	436	SER	2.2
1	A	689	ASN	2.2
1	D	635	GLN	2.2
1	A	687	ASP	2.2
1	C	819	ASP	2.2
1	B	435	GLY	2.1
1	D	435	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	686	CYS	2.1
1	C	550	ALA	2.0
1	B	437	LYS	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	SO4	B	7	5/5	0.81	0.34	35,36,39,39	5
2	SO4	A	5	5/5	0.88	0.41	55,56,60,60	5
2	SO4	B	8	5/5	0.88	0.22	30,32,35,36	5
2	SO4	A	4	5/5	0.89	0.21	33,35,36,39	5
2	SO4	B	9	5/5	0.90	0.20	33,33,36,36	5
3	GOL	D	5	6/6	0.90	0.24	29,34,43,49	0
2	SO4	D	3	5/5	0.91	0.21	34,35,36,37	5
2	SO4	C	4	5/5	0.92	0.21	33,33,35,35	5
2	SO4	D	2	5/5	0.92	0.21	40,40,41,42	5
2	SO4	C	6	5/5	0.93	0.32	51,54,56,57	5
3	GOL	C	8	6/6	0.93	0.25	34,34,36,39	0
2	SO4	B	6	5/5	0.93	0.16	42,42,43,44	5
3	GOL	A	7	6/6	0.94	0.28	39,40,43,49	0
3	GOL	B	10	6/6	0.94	0.25	36,39,43,50	0
2	SO4	A	6	5/5	0.94	0.34	59,59,62,63	5
2	SO4	D	1	5/5	0.94	0.14	34,38,39,42	5
2	SO4	B	5	5/5	0.95	0.14	46,48,49,51	5
2	SO4	C	3	5/5	0.95	0.13	47,49,50,50	5
2	SO4	A	2	5/5	0.95	0.17	36,36,38,38	5
2	SO4	C	5	5/5	0.95	0.17	37,38,40,41	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	3	5/5	0.96	0.09	41,41,42,44	5
2	SO4	D	4	5/5	0.97	0.18	49,54,54,54	5
2	SO4	C	2	5/5	0.97	0.12	30,31,35,36	5
2	SO4	B	3	5/5	0.97	0.14	18,18,21,21	5
2	SO4	A	1	5/5	0.97	0.18	25,28,29,30	5
2	SO4	C	1	5/5	0.97	0.14	42,42,43,46	5
2	SO4	B	4	5/5	0.98	0.08	25,26,29,31	5
2	SO4	C	7	5/5	0.98	0.12	32,34,37,37	5

6.5 Other polymers (i)

There are no such residues in this entry.