Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 02:07 AM EDT

PDB ID	:	4H15
Title	:	Crystal Structure of a short chain alcohol dehydrogenase-related dehydrogenase (target ID NYSGRC-011812) from Sinorhizobium meliloti 1021 in space group P21
Authors	:	Ghosh, A.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-09-10
Resolution	:	1.45 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 (i) 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 (i)) were used in the production of this report:

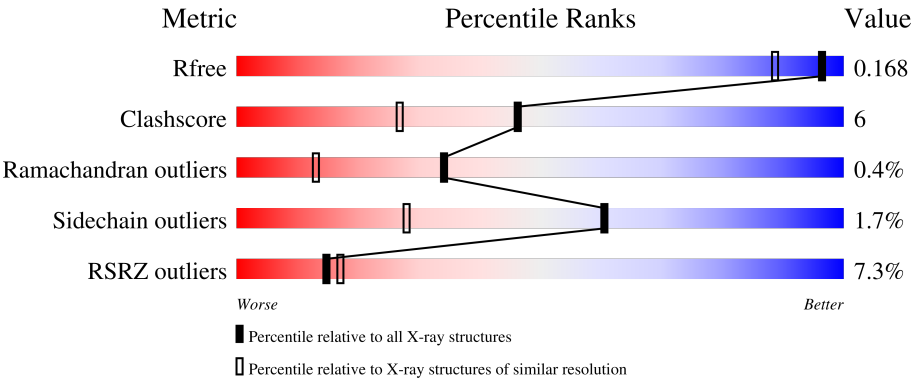
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	261	7% 89% 11%
1	B	261	8% 89% 11%
1	C	261	5% 92% 7%
1	D	261	8% 90% 8%

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
3	CL	A	310[A]	-	-	X	-
3	CL	C	306[A]	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9061 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 Short chain alcohol dehydrogenase-related dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	Se	0	14	0
			1986	1253	342	381	1	9			
1	B	261	Total	C	N	O	S	Se	0	18	0
			1996	1265	338	383	1	9			
1	C	261	Total	C	N	O	S	Se	0	12	0
			1968	1241	339	378	1	9			
1	D	261	Total	C	N	O	S	Se	0	11	0
			1967	1244	337	377	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q92YJ2
A	0	MSE	-	EXPRESSION TAG	UNP Q92YJ2
B	-1	SER	-	EXPRESSION TAG	UNP Q92YJ2
B	0	MSE	-	EXPRESSION TAG	UNP Q92YJ2
C	-1	SER	-	EXPRESSION TAG	UNP Q92YJ2
C	0	MSE	-	EXPRESSION TAG	UNP Q92YJ2
D	-1	SER	-	EXPRESSION TAG	UNP Q92YJ2
D	0	MSE	-	EXPRESSION TAG	UNP Q92YJ2

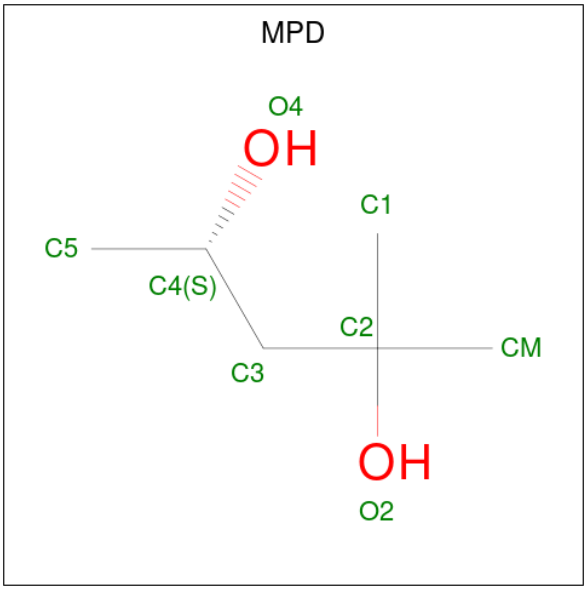
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	1
			4	4		
2	D	4	Total	Ca	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total Cl 14 14	0	1
3	B	9	Total Cl 9 9	0	2
3	C	9	Total Cl 10 10	0	3
3	D	8	Total Cl 9 9	0	1

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0

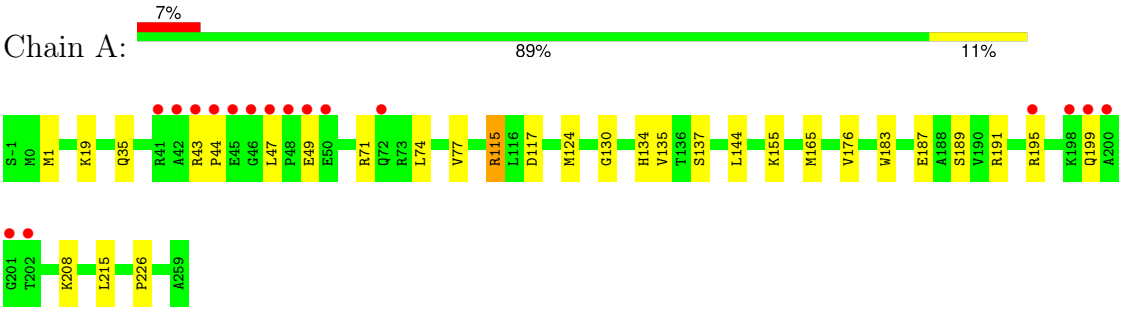
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	228	Total O 239 239	0	11
5	B	221	Total O 237 237	0	15
5	C	257	Total O 266 266	0	9
5	D	235	Total O 252 252	0	17

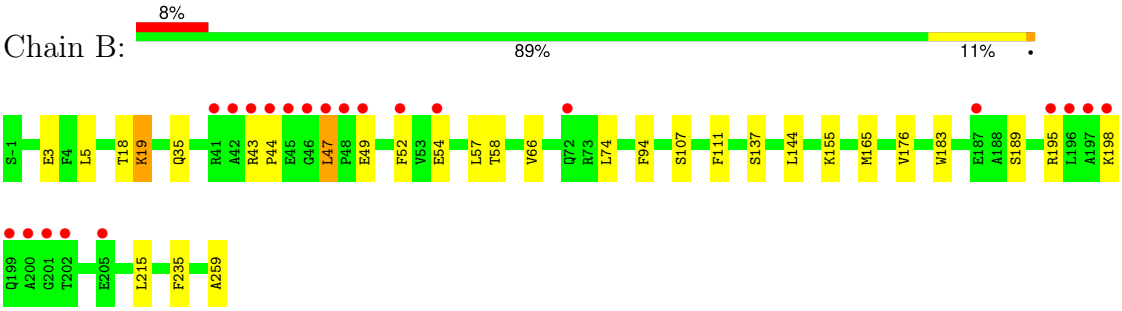
3 Residue-property plots (i)

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.

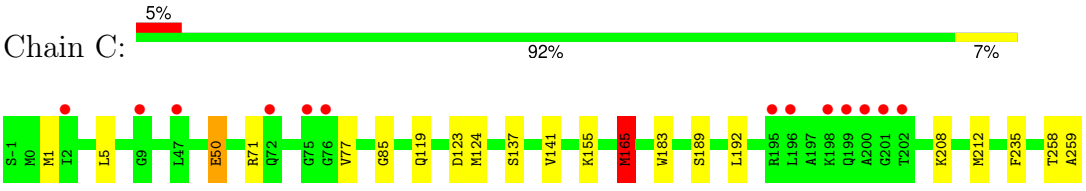
• Molecule 1: Short chain alcohol dehydrogenase-related dehydrogenase



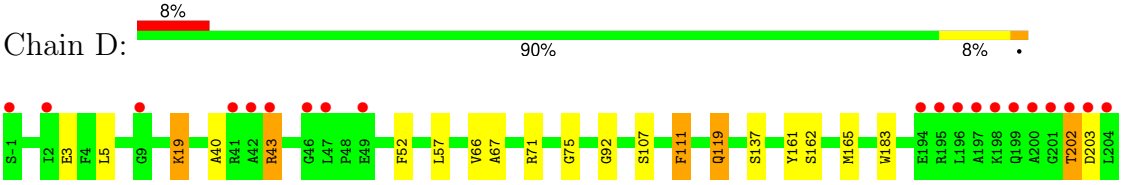
• Molecule 1: Short chain alcohol dehydrogenase-related dehydrogenase



• Molecule 1: Short chain alcohol dehydrogenase-related dehydrogenase



• Molecule 1: Short chain alcohol dehydrogenase-related dehydrogenase




E205
K209
M212
P223
F235
T258
A259

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.30Å 119.14Å 67.16Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	27.79 – 1.45 27.79 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.79-1.45) 98.1 (27.79-1.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.13 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.150 , 0.167 0.150 , 0.168	Depositor DCC
R_{free} test set	8550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9061	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: CA, CL, MPD

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	0.33	0/2045	0.53	0/2756
1	B	0.35	0/2072	0.56	0/2796
1	C	0.35	0/2024	0.56	2/2730 (0.1%)
1	D	0.37	0/2016	0.56	0/2720
All	All	0.35	0/8157	0.55	2/11002 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	165[A]	MSE	CG-SE-CE	-5.18	87.50	98.90
1	C	165[B]	MSE	CG-SE-CE	-5.18	87.50	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1986	0	2079	24	0
1	B	1996	0	2095	34	0
1	C	1968	0	2057	17	0
1	D	1967	0	2041	27	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	14	0	0	6	0
3	B	9	0	0	0	0
3	C	10	0	0	5	0
3	D	9	0	0	1	0
4	A	24	0	42	2	0
4	B	24	0	42	4	0
4	C	32	0	56	5	0
4	D	16	0	28	0	0
5	A	239	0	0	5	0
5	B	237	0	0	4	0
5	C	266	0	0	2	0
5	D	252	0	0	5	0
All	All	9061	0	8440	104	0

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

All (104) 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)
3:A:309:CL:CL	5:D:611:HOH:O	2.24	0.92
1:B:44:PRO:HG2	1:B:47:LEU:HD11	1.57	0.86
3:C:306[A]:CL:CL	5:C:656:HOH:O	2.37	0.79
3:A:312:CL:CL	5:A:488[A]:HOH:O	2.38	0.79
1:C:155:LYS:HZ1	4:C:316:MPD:H13	1.51	0.76
1:C:71[B]:ARG:NH2	1:C:123:ASP:OD2	2.17	0.72
1:B:155:LYS:HZ1	4:B:315:MPD:H13	1.53	0.72
1:D:75:GLY:O	5:D:575[A]:HOH:O	2.07	0.72
1:A:44:PRO:HB2	1:A:47:LEU:HD13	1.73	0.71
1:D:71:ARG:HH22	1:D:119:GLN:HG3	1.55	0.70
3:A:310[A]:CL:CL	5:B:545[A]:HOH:O	2.47	0.69
1:D:67:ALA:HB1	1:D:119:GLN:HG2	1.73	0.68
1:B:155:LYS:NZ	4:B:315:MPD:H13	2.09	0.68
3:C:306[A]:CL:CL	5:C:508:HOH:O	2.49	0.67
1:C:183:TRP:HE1	1:C:189[B]:SER:HB2	1.61	0.66
1:D:71:ARG:NH2	1:D:119:GLN:HG3	2.13	0.63
1:C:5:LEU:HD11	1:C:235:PHE:HA	1.83	0.61
1:B:43:ARG:HH12	1:B:49:GLU:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:CL:CL	4:C:315:MPD:H52	2.38	0.60
1:B:94:PHE:CG	1:D:165[B]:MSE:SE	3.05	0.59
1:B:195:ARG:HA	1:B:198:LYS:HE2	1.83	0.59
1:B:144[A]:LEU:HD11	1:B:215:LEU:HD23	1.84	0.59
1:A:144[B]:LEU:HD11	1:A:215:LEU:HD23	1.84	0.58
1:D:202:THR:OG1	1:D:203:ASP:N	2.37	0.58
1:D:161:TYR:O	1:D:165[B]:MSE:HG2	2.03	0.58
1:C:50:GLU:H	1:C:50:GLU:CD	2.07	0.57
1:A:117:ASP:HB3	1:A:165[B]:MSE:HE1	1.85	0.57
1:D:5:LEU:HD11	1:D:235:PHE:HA	1.87	0.56
1:D:57[A]:LEU:HD21	1:D:66:VAL:HG21	1.88	0.56
1:B:94:PHE:CB	1:D:165[B]:MSE:SE	3.04	0.56
1:C:155:LYS:NZ	4:C:316:MPD:H13	2.18	0.56
1:B:43:ARG:HD3	1:B:44:PRO:HD2	1.87	0.56
1:A:77:VAL:O	1:A:124[B]:MSE:HE3	2.07	0.55
1:C:71[B]:ARG:NH1	1:C:119:GLN:O	2.40	0.55
1:A:135:VAL:HG11	4:A:317:MPD:HM1	1.89	0.55
1:B:94:PHE:CE2	1:D:165[B]:MSE:HE1	2.41	0.55
1:B:43:ARG:CZ	1:B:52:PHE:HB2	2.37	0.55
1:D:162:SER:O	1:D:165[B]:MSE:HB2	2.06	0.54
1:D:19:LYS:HG2	5:D:732:HOH:O	2.06	0.54
1:A:124[A]:MSE:HE2	1:A:130:GLY:HA3	1.90	0.53
1:D:43:ARG:NE	5:D:625:HOH:O	2.42	0.53
1:B:94:PHE:CD2	1:D:165[B]:MSE:HE1	2.44	0.53
1:A:183:TRP:HE1	1:A:189[B]:SER:HB3	1.73	0.52
1:C:77:VAL:O	1:C:124[B]:MSE:HE3	2.11	0.51
1:A:183:TRP:HE1	1:A:189[A]:SER:CB	2.24	0.51
1:C:183:TRP:HE1	1:C:189[B]:SER:CB	2.23	0.51
4:C:313:MPD:HM1	4:C:315:MPD:H53	1.92	0.50
1:A:35[A]:GLN:HG2	1:A:74:LEU:HD22	1.94	0.49
1:D:71:ARG:HH22	1:D:119:GLN:CG	2.24	0.49
1:A:19:LYS:HD3	3:A:306:CL:CL	2.49	0.49
1:B:5:LEU:HD11	1:B:235:PHE:HA	1.95	0.49
1:A:183:TRP:HE1	1:A:189[B]:SER:CB	2.26	0.49
1:D:107[B]:SER:HA	1:D:111[B]:PHE:HB2	1.95	0.49
1:A:187:GLU:HG3	3:A:303:CL:CL	2.50	0.48
1:A:115[A]:ARG:NH1	5:A:471:HOH:O	2.41	0.48
1:A:183:TRP:HE1	1:A:189[A]:SER:HB2	1.78	0.48
1:D:67:ALA:CB	1:D:119:GLN:HG2	2.41	0.47
1:D:107[B]:SER:HA	1:D:111[B]:PHE:CD2	2.49	0.47
1:B:183:TRP:HE1	1:B:189:SER:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165[A]:MSE:HE3	1:C:165[A]:MSE:HB2	1.46	0.47
1:D:183:TRP:HZ3	1:D:212:MSE:HG3	1.80	0.46
1:A:155:LYS:NZ	4:A:317:MPD:O4	2.45	0.46
1:B:107[A]:SER:HA	1:B:111[A]:PHE:HB2	1.97	0.46
3:D:306:CL:CL	3:D:310:CL:CL	3.08	0.46
1:B:183:TRP:HE1	1:B:189:SER:CB	2.29	0.46
1:D:203:ASP:OD1	1:D:205:GLU:N	2.49	0.46
1:A:183:TRP:HH2	1:A:208:LYS:HG3	1.81	0.46
1:B:35[A]:GLN:HG2	1:B:74:LEU:HD22	1.98	0.46
1:A:71:ARG:NH1	5:A:626:HOH:O	2.26	0.45
1:B:35[A]:GLN:NE2	5:B:618:HOH:O	2.43	0.45
1:B:58:THR:HB	1:B:107[C]:SER:OG	2.16	0.45
3:C:305:CL:CL	3:C:309:CL:CL	3.09	0.45
1:C:208:LYS:HG2	1:C:212[B]:MSE:SE	2.67	0.45
1:B:18:THR:O	1:B:19:LYS:NZ	2.37	0.45
1:B:3:GLU:OE1	1:C:1:MSE:HE3	2.18	0.44
1:D:183:TRP:CD2	1:D:223:PRO:HB3	2.53	0.44
1:B:18:THR:O	1:B:19:LYS:HD2	2.18	0.44
1:A:199:GLN:NE2	5:A:578:HOH:O	2.35	0.43
1:D:40:ALA:HB3	1:D:52[B]:PHE:CE1	2.53	0.43
1:C:85:GLY:HA3	4:C:316:MPD:H12	2.01	0.43
1:A:165[B]:MSE:HG2	1:A:176:VAL:HG21	2.01	0.42
1:B:18:THR:HG23	5:B:479:HOH:O	2.19	0.42
1:A:191:ARG:O	1:A:195:ARG:HG3	2.19	0.42
1:B:107[A]:SER:HA	1:B:111[A]:PHE:CD2	2.54	0.42
1:C:77:VAL:HG13	1:C:124[A]:MSE:SE	2.69	0.42
1:D:92:GLY:O	5:D:650:HOH:O	2.22	0.42
1:A:134:HIS:HE1	1:A:165[A]:MSE:HE2	1.84	0.42
1:B:54:GLU:O	1:B:54:GLU:HG3	2.19	0.42
1:B:155:LYS:HZ1	4:B:315:MPD:C1	2.26	0.42
1:B:165[A]:MSE:HG2	1:B:176:VAL:HG21	2.01	0.42
1:B:47:LEU:H	1:B:47:LEU:HG	1.47	0.42
1:A:183:TRP:CH2	1:A:208:LYS:HG3	2.55	0.41
4:B:315:MPD:H4	4:B:315:MPD:H11	1.54	0.41
1:B:94:PHE:HB3	1:D:165[B]:MSE:SE	2.70	0.41
1:C:259:ALA:O	3:C:307[B]:CL:CL	2.75	0.41
3:A:310[A]:CL:CL	1:B:259:ALA:O	2.76	0.41
1:C:141:VAL:O	1:D:258:THR:HA	2.21	0.41
1:A:1:MSE:HE2	1:D:3:GLU:HG3	2.03	0.41
1:A:226:PRO:HD2	5:A:510:HOH:O	2.21	0.41
1:B:43:ARG:HA	1:B:44:PRO:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HA	5:B:514:HOH:O	2.21	0.40
1:B:47:LEU:HD22	1:B:52:PHE:CE1	2.56	0.40
1:B:57:LEU:HD21	1:B:66:VAL:HG21	2.03	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	274/261 (105%)	270 (98%)	3 (1%)	1 (0%)	34	13
1	B	278/261 (106%)	274 (99%)	3 (1%)	1 (0%)	34	13
1	C	272/261 (104%)	267 (98%)	4 (2%)	1 (0%)	34	13
1	D	270/261 (103%)	267 (99%)	2 (1%)	1 (0%)	34	13
All	All	1094/1044 (105%)	1078 (98%)	12 (1%)	4 (0%)	34	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	SER
1	A	137	SER
1	B	137	SER
1	C	137	SER

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	211/190 (111%)	207 (98%)	4 (2%)	57 23
1	B	215/190 (113%)	213 (99%)	2 (1%)	78 57
1	C	209/190 (110%)	204 (98%)	5 (2%)	49 16
1	D	207/190 (109%)	201 (97%)	6 (3%)	42 10
All	All	842/760 (111%)	825 (98%)	17 (2%)	60 22

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	49	GLU
1	A	115[A]	ARG
1	A	115[B]	ARG
1	B	19	LYS
1	B	47	LEU
1	C	50	GLU
1	C	165[A]	MSE
1	C	165[B]	MSE
1	C	192[A]	LEU
1	C	192[B]	LEU
1	D	19	LYS
1	D	43	ARG
1	D	111[A]	PHE
1	D	111[B]	PHE
1	D	119	GLN
1	D	202	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 54 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
4	MPD	B	313	-	7,7,7	0.33	0	9,10,10	0.31	0
4	MPD	D	314	-	7,7,7	0.28	0	9,10,10	0.33	0
4	MPD	C	316	-	7,7,7	0.38	0	9,10,10	0.71	0
4	MPD	A	318	-	7,7,7	0.25	0	9,10,10	0.33	0
4	MPD	D	313	-	7,7,7	0.28	0	9,10,10	0.37	0
4	MPD	B	314	-	7,7,7	0.24	0	9,10,10	0.29	0
4	MPD	A	317	-	7,7,7	0.32	0	9,10,10	0.27	0
4	MPD	C	315	-	7,7,7	0.20	0	9,10,10	0.45	0
4	MPD	C	313	-	7,7,7	0.25	0	9,10,10	0.28	0
4	MPD	B	315	-	7,7,7	0.26	0	9,10,10	0.65	0
4	MPD	A	316	-	7,7,7	0.34	0	9,10,10	0.34	0
4	MPD	C	314	-	7,7,7	0.27	0	9,10,10	0.19	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
4	MPD	B	313	-	-	0/5/5/5	-
4	MPD	D	314	-	-	0/5/5/5	-
4	MPD	C	316	-	-	5/5/5/5	-
4	MPD	A	318	-	-	0/5/5/5	-
4	MPD	D	313	-	-	0/5/5/5	-
4	MPD	B	314	-	-	0/5/5/5	-
4	MPD	A	317	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	C	315	-	-	2/5/5/5	-
4	MPD	C	313	-	-	0/5/5/5	-
4	MPD	B	315	-	-	2/5/5/5	-
4	MPD	A	316	-	-	0/5/5/5	-
4	MPD	C	314	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	316	MPD	C1-C2-C3-C4
4	C	316	MPD	CM-C2-C3-C4
4	C	316	MPD	C2-C3-C4-O4
4	C	316	MPD	C2-C3-C4-C5
4	B	315	MPD	O2-C2-C3-C4
4	C	315	MPD	C2-C3-C4-C5
4	C	316	MPD	O2-C2-C3-C4
4	B	315	MPD	C2-C3-C4-O4
4	C	315	MPD	C2-C3-C4-O4
4	C	314	MPD	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	316	MPD	3	0
4	A	317	MPD	2	0
4	C	315	MPD	2	0
4	C	313	MPD	1	0
4	B	315	MPD	4	0

5.7 Other polymers

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	255/261 (97%)	0.21	17 (6%)	17	19	5, 12, 37, 61	0
1	B	255/261 (97%)	0.38	22 (8%)	10	12	4, 10, 44, 74	0
1	C	255/261 (97%)	0.07	13 (5%)	28	30	4, 11, 31, 54	0
1	D	255/261 (97%)	0.30	22 (8%)	10	12	4, 12, 42, 64	0
All	All	1020/1044 (97%)	0.24	74 (7%)	15	17	4, 11, 39, 74	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	LEU	11.9
1	B	44	PRO	10.1
1	A	46	GLY	9.5
1	D	200	ALA	8.8
1	B	43	ARG	8.6
1	B	46	GLY	7.7
1	D	204	LEU	7.6
1	B	42	ALA	7.2
1	A	47	LEU	6.8
1	B	200	ALA	6.6
1	D	201	GLY	6.4
1	D	199	GLN	6.2
1	A	45	GLU	6.0
1	B	45	GLU	5.8
1	D	198	LYS	5.7
1	A	43	ARG	5.4
1	D	196	LEU	5.4
1	A	44	PRO	5.1
1	B	198	LYS	5.1
1	A	199	GLN	4.3
1	A	200	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	200	ALA	4.3
1	D	205	GLU	4.2
1	B	199	GLN	4.2
1	B	48	PRO	4.1
1	B	49	GLU	4.1
1	B	201	GLY	4.0
1	D	202	THR	4.0
1	B	197	ALA	4.0
1	A	198	LYS	3.9
1	D	197	ALA	3.9
1	B	41	ARG	3.7
1	D	195	ARG	3.6
1	B	195	ARG	3.6
1	D	46	GLY	3.5
1	C	199	GLN	3.4
1	D	9	GLY	3.4
1	C	201	GLY	3.3
1	A	42	ALA	3.3
1	D	203	ASP	3.3
1	B	202	THR	3.2
1	A	201	GLY	3.1
1	C	198	LYS	3.0
1	A	41	ARG	3.0
1	A	72	GLN	3.0
1	C	196	LEU	3.0
1	A	195	ARG	2.9
1	A	49	GLU	2.8
1	C	75	GLY	2.8
1	C	2	ILE	2.8
1	D	209	LYS	2.8
1	C	202	THR	2.7
1	D	2	ILE	2.7
1	C	76	GLY	2.7
1	B	196	LEU	2.6
1	C	195	ARG	2.6
1	B	187	GLU	2.5
1	A	202	THR	2.4
1	B	205	GLU	2.4
1	A	48	PRO	2.4
1	D	43	ARG	2.4
1	D	42	ALA	2.3
1	D	47	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	9	GLY	2.3
1	B	54	GLU	2.3
1	D	194	GLU	2.2
1	A	50	GLU	2.2
1	B	72	GLN	2.2
1	D	-1	SER	2.1
1	C	72	GLN	2.1
1	D	41	ARG	2.1
1	D	49	GLU	2.1
1	B	52	PHE	2.0
1	C	47	LEU	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
4	MPD	C	315	8/8	0.73	0.23	24,35,44,46	0
4	MPD	C	314	8/8	0.76	0.20	20,28,33,39	0
4	MPD	C	316	8/8	0.77	0.24	18,36,50,55	0
2	CA	C	303	1/1	0.79	0.16	58,58,58,58	0
4	MPD	D	314	8/8	0.83	0.13	22,28,41,50	0
3	CL	B	308[B]	1/1	0.84	0.16	27,27,27,27	1
4	MPD	B	314	8/8	0.84	0.16	26,30,37,44	0
4	MPD	A	317	8/8	0.85	0.17	9,40,47,49	0
4	MPD	B	315	8/8	0.86	0.24	17,31,42,61	0
4	MPD	A	318	8/8	0.88	0.13	19,24,34,44	0
3	CL	A	310[A]	1/1	0.89	0.11	27,27,27,27	1
2	CA	D	304	1/1	0.90	0.33	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	B	310	1/1	0.90	0.13	39,39,39,39	1
3	CL	C	307[A]	1/1	0.91	0.20	25,25,25,25	1
3	CL	C	307[B]	1/1	0.91	0.20	27,27,27,27	1
3	CL	B	307[B]	1/1	0.94	0.10	26,26,26,26	1
3	CL	D	311	1/1	0.94	0.20	38,38,38,38	0
2	CA	C	302[B]	1/1	0.94	0.10	18,18,18,18	1
3	CL	A	305	1/1	0.94	0.16	38,38,38,38	0
2	CA	C	302[A]	1/1	0.94	0.10	25,25,25,25	1
3	CL	A	309	1/1	0.95	0.10	27,27,27,27	0
3	CL	A	308	1/1	0.95	0.17	43,43,43,43	0
3	CL	C	308[A]	1/1	0.95	0.10	41,41,41,41	1
3	CL	A	314	1/1	0.95	0.07	13,13,13,13	1
3	CL	C	312	1/1	0.96	0.09	21,21,21,21	1
2	CA	D	303	1/1	0.96	0.12	19,19,19,19	1
4	MPD	C	313	8/8	0.96	0.10	8,13,21,27	0
4	MPD	A	316	8/8	0.96	0.10	7,15,19,27	0
3	CL	A	313	1/1	0.96	0.06	22,22,22,22	0
3	CL	A	307	1/1	0.96	0.07	21,21,21,21	1
4	MPD	D	313	8/8	0.96	0.09	8,14,20,20	0
4	MPD	B	313	8/8	0.96	0.09	8,13,21,27	0
3	CL	B	306	1/1	0.97	0.09	24,24,24,24	0
3	CL	B	311	1/1	0.97	0.08	11,11,11,11	1
3	CL	D	310	1/1	0.97	0.07	25,25,25,25	0
3	CL	B	312	1/1	0.97	0.07	16,16,16,16	1
3	CL	C	305	1/1	0.97	0.15	32,32,32,32	0
3	CL	C	306[A]	1/1	0.97	0.07	16,16,16,16	1
2	CA	D	302	1/1	0.97	0.10	16,16,16,16	1
2	CA	B	302	1/1	0.97	0.07	17,17,17,17	1
3	CL	A	304	1/1	0.98	0.07	19,19,19,19	0
2	CA	C	301	1/1	0.98	0.07	14,14,14,14	0
3	CL	A	312	1/1	0.98	0.13	39,39,39,39	0
3	CL	D	312	1/1	0.98	0.08	14,14,14,14	1
3	CL	B	309	1/1	0.98	0.05	17,17,17,17	0
2	CA	B	303	1/1	0.98	0.14	28,28,28,28	1
2	CA	D	301	1/1	0.98	0.06	14,14,14,14	0
3	CL	C	309	1/1	0.98	0.05	23,23,23,23	0
3	CL	D	309[B]	1/1	0.99	0.06	27,27,27,27	1
3	CL	A	311	1/1	0.99	0.04	13,13,13,13	0
3	CL	A	315	1/1	0.99	0.06	10,10,10,10	0
3	CL	A	303	1/1	0.99	0.04	20,20,20,20	0
3	CL	A	306	1/1	0.99	0.25	34,34,34,34	0
3	CL	D	306	1/1	0.99	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	D	308	1/1	0.99	0.03	20,20,20,20	0
3	CL	D	309[A]	1/1	0.99	0.06	17,17,17,17	1
3	CL	B	304	1/1	1.00	0.04	10,10,10,10	0
3	CL	D	307	1/1	1.00	0.04	10,10,10,10	0
3	CL	B	305	1/1	1.00	0.04	11,11,11,11	0
2	CA	B	301	1/1	1.00	0.04	9,9,9,9	0
3	CL	A	302	1/1	1.00	0.03	9,9,9,9	0
3	CL	C	304	1/1	1.00	0.04	6,6,6,6	0
3	CL	C	310	1/1	1.00	0.04	18,18,18,18	0
3	CL	C	311	1/1	1.00	0.03	10,10,10,10	0
2	CA	A	301	1/1	1.00	0.04	7,7,7,7	0
3	CL	D	305	1/1	1.00	0.03	7,7,7,7	0

6.5 Other polymers (i)

There are no such residues in this entry.