Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 06:13 PM JST

PDB ID	:	6LYN
Title	:	CD146 D4-D5/AA98 Fab
Authors	:	Chen, X.; Yan, X.
Deposited on	:	2020-02-14
Resolution	:	2.78 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:

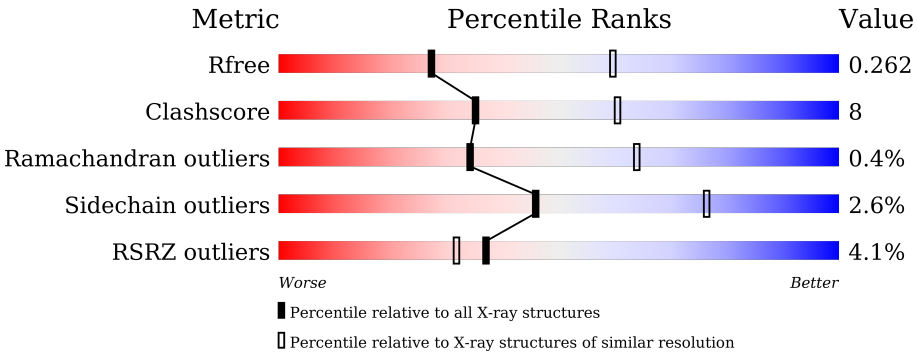
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	217	2% 76% 22% ·
1	H	217	2% 80% 17% ··
2	B	218	4% 81% 19%
2	L	218	5% 81% 18%
3	C	184	5% 76% 22% ··
3	D	184	7% 73% 24% ··

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9727 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 AA98 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	2	0
			1640	1050	264	320	6			
1	H	212	Total	C	N	O	S	0	1	0
			1625	1042	259	318	6			

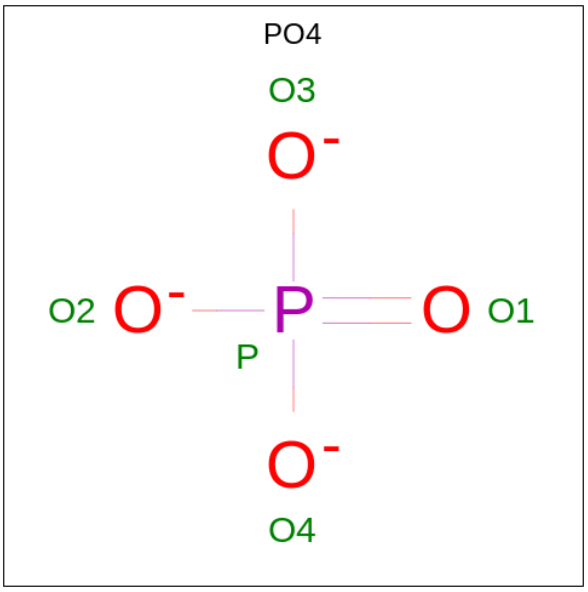
- Molecule 2 is a protein called AA98 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	1	0
			1693	1055	287	343	8			
2	L	217	Total	C	N	O	S	0	1	0
			1687	1054	286	340	7			

- Molecule 3 is a protein called Cell surface glycoprotein MUC18.

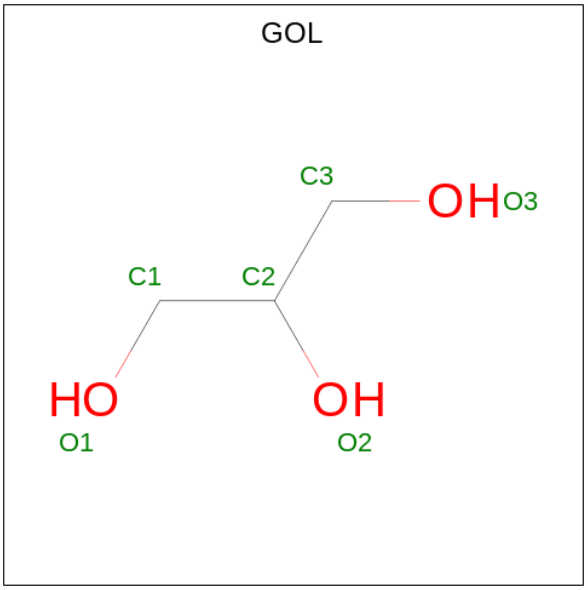
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1418	885	247	280	6			
3	D	182	Total	C	N	O	S	0	0	0
			1410	881	245	278	6			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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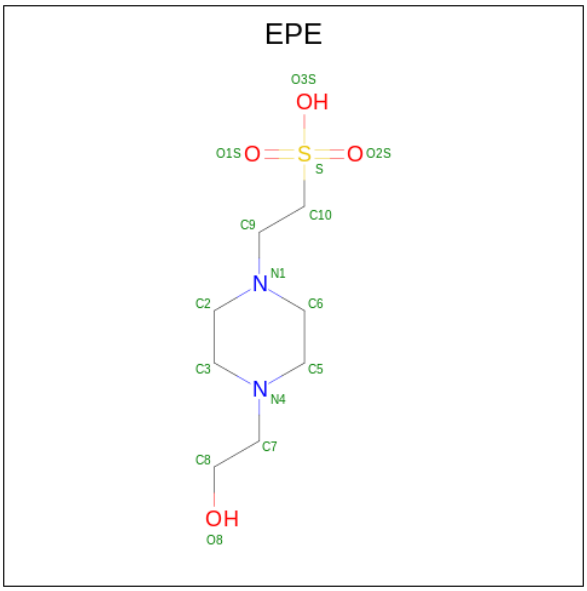
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

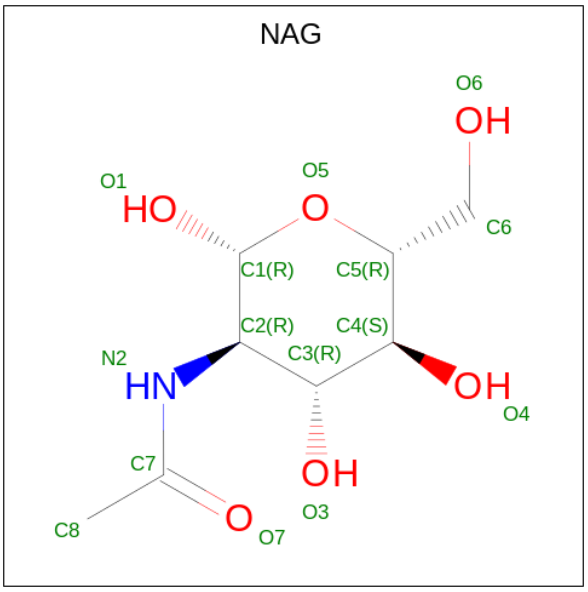
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	D	2	Total Cl 2 2	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O S 15 8 2 4 1	0	0
7	L	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0

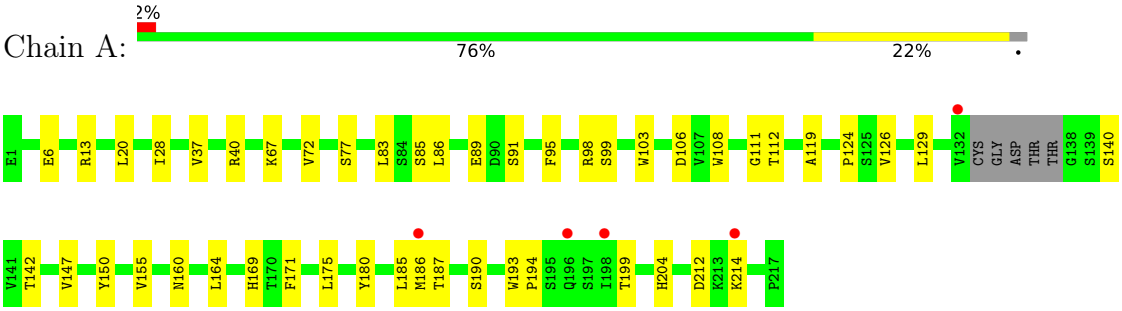
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	25	Total O 25 25	0	0
9	B	21	Total O 21 21	0	0
9	C	17	Total O 17 17	0	0
9	L	25	Total O 25 25	0	0
9	D	15	Total O 15 15	0	0
9	H	33	Total O 33 33	0	0

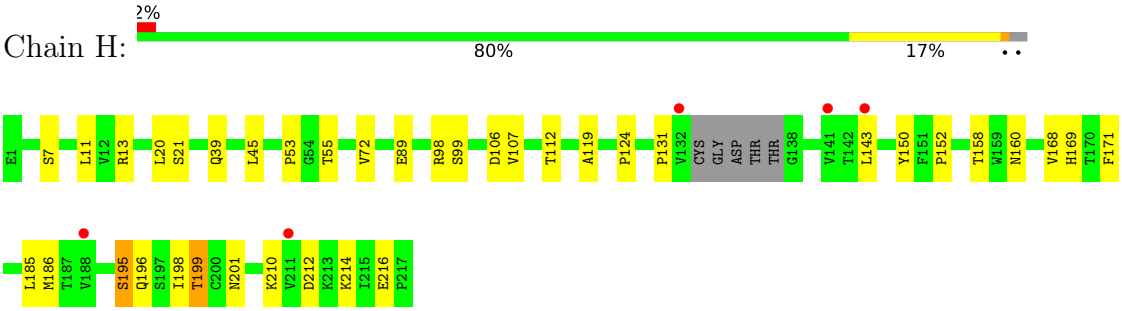
3 Residue-property plots (i)

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.

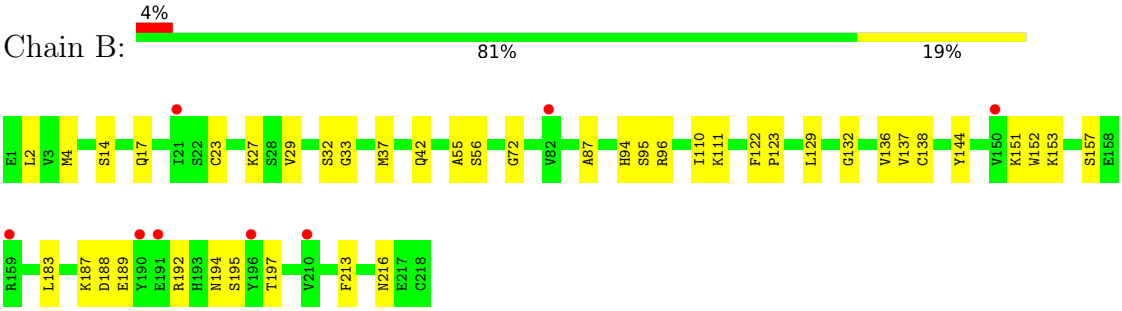
• Molecule 1: AA98 Fab heavy chain



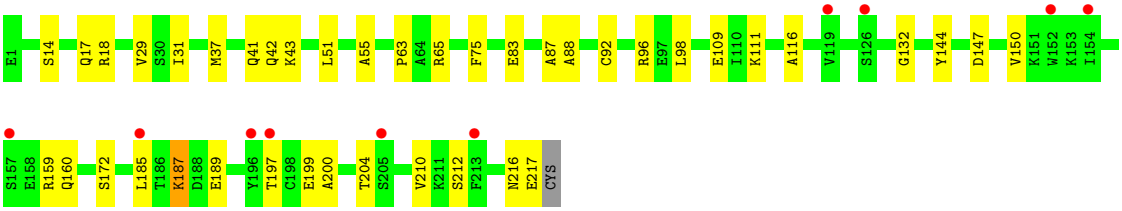
• Molecule 1: AA98 Fab heavy chain



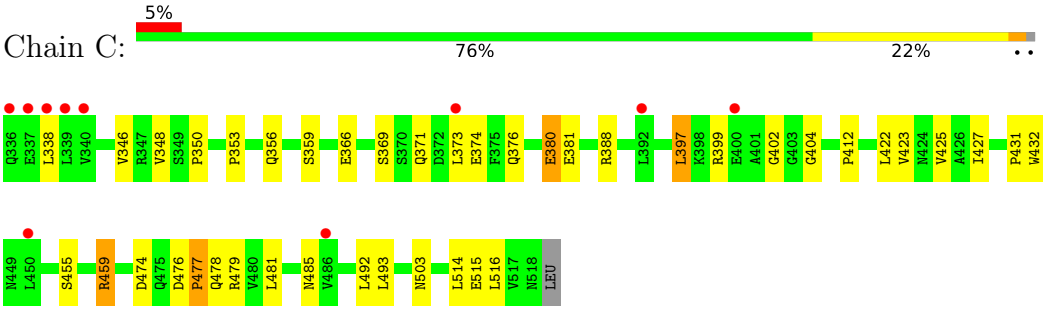
• Molecule 2: AA98 Fab light chain



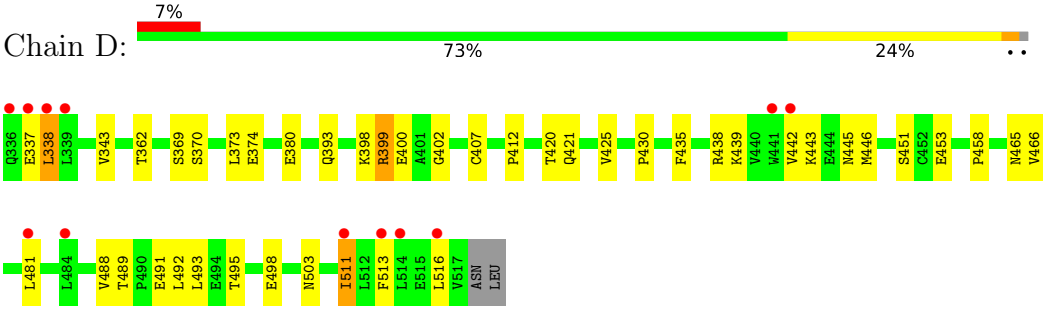
• Molecule 2: AA98 Fab light chain



• Molecule 3: Cell surface glycoprotein MUC18



• Molecule 3: Cell surface glycoprotein MUC18



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.20Å 88.39Å 94.64Å 90.00° 89.93° 90.00°	Depositor
Resolution (Å)	29.71 – 2.78 29.71 – 2.78	Depositor EDS
% Data completeness (in resolution range)	87.5 (29.71-2.78) 87.3 (29.71-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.217 , 0.262 0.217 , 0.262	Depositor DCC
R_{free} test set	1583 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l 0.008 for -k,-h,-l 0.460 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9727	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: NAG, CL, EPE, PO4, 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	0.26	0/1684	0.48	0/2298
1	H	0.26	0/1672	0.48	0/2281
2	B	0.26	0/1736	0.46	0/2356
2	L	0.27	0/1730	0.49	1/2349 (0.0%)
3	C	0.26	0/1444	0.52	0/1968
3	D	0.26	0/1436	0.50	0/1957
All	All	0.26	0/9702	0.49	1/13209 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	185	LEU	CA-CB-CG	5.26	127.41	115.30

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	1640	0	1610	28	0
1	H	1625	0	1595	23	0
2	B	1693	0	1624	28	0
2	L	1687	0	1626	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1418	0	1395	27	0
3	D	1410	0	1389	28	0
4	A	5	0	0	0	0
4	H	5	0	0	0	0
5	A	6	0	8	2	0
5	C	12	0	16	3	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
7	B	15	0	17	3	0
7	L	15	0	17	2	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
9	A	25	0	0	0	0
9	B	21	0	0	0	0
9	C	17	0	0	0	0
9	D	15	0	0	1	0
9	H	33	0	0	1	0
9	L	25	0	0	0	0
All	All	9727	0	9349	155	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 8.

All (155) 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:D:439:LYS:HG2	3:D:513:PHE:HB2	1.61	0.82
3:C:369:SER:HB3	3:C:373:LEU:HD11	1.63	0.78
2:B:153:LYS:HB2	2:B:197:THR:HB	1.69	0.74
3:D:493:LEU:HD22	3:D:516:LEU:HD12	1.72	0.71
3:C:350:PRO:HG2	3:C:353:PRO:HG3	1.72	0.70
2:L:116:ALA:HB2	2:L:204:THR:HG21	1.73	0.70
1:A:160:ASN:HD22	1:A:164:LEU:HD23	1.56	0.69
3:D:458:PRO:O	3:D:503:ASN:ND2	2.26	0.69
1:H:124:PRO:HB3	1:H:150:TYR:HB3	1.77	0.67
3:D:488:VAL:HG13	3:D:493:LEU:HD11	1.77	0.66
1:A:199:THR:HG1	1:A:214:LYS:HZ2	1.43	0.66
3:C:476:ASP:HB3	3:C:479:ARG:HB2	1.79	0.64
2:L:43[A]:LYS:HD2	2:L:88:ALA:HB2	1.80	0.64
1:A:129:LEU:HD13	2:B:137:VAL:HG11	1.79	0.63
3:D:362:THR:OG1	3:D:393:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:PRO:HG3	2:L:65:ARG:HH21	1.64	0.63
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.83	0.61
2:L:14:SER:HA	2:L:111:LYS:HB2	1.82	0.61
1:A:13[A]:ARG:NH1	1:A:119:ALA:O	2.28	0.61
3:C:397:LEU:HD12	3:C:427:ILE:HD11	1.82	0.60
3:D:465:ASN:ND2	9:D:701:HOH:O	2.31	0.60
1:A:142:THR:HG23	1:A:187:THR:HG22	1.83	0.60
3:C:399:ARG:HG3	5:C:604:GOL:H12	1.83	0.60
2:L:150:VAL:HG12	2:L:200:ALA:HB2	1.84	0.59
1:H:171:PHE:HE2	1:H:185:LEU:HD23	1.67	0.59
1:A:103:TRP:HB2	2:B:95:SER:HB2	1.84	0.59
7:B:301:EPE:H72	3:C:422:LEU:HD23	1.83	0.58
1:A:28:ILE:HA	5:A:302:GOL:H12	1.85	0.58
2:L:132:GLY:HA2	2:L:187:LYS:HD3	1.86	0.56
3:D:443:LYS:H	3:D:446:MET:CE	2.18	0.56
3:C:348:VAL:HG21	3:C:423:VAL:HB	1.86	0.56
3:C:402:GLY:HA2	3:C:425:VAL:HG23	1.86	0.56
2:B:136:VAL:HG12	2:B:183:LEU:HB3	1.88	0.56
1:A:199:THR:HG21	1:A:212:ASP:HB2	1.88	0.55
2:B:2:LEU:HG	2:B:27:LYS:HE2	1.89	0.55
2:B:151:LYS:HE2	2:B:153:LYS:HE3	1.89	0.54
3:D:498:GLU:HG2	3:D:511:ILE:HD12	1.90	0.54
1:A:126:VAL:HG22	1:A:147:VAL:HG12	1.90	0.54
2:L:29:VAL:HG21	2:L:37:MET:HG2	1.90	0.54
1:H:158:THR:OG1	1:H:201:ASN:ND2	2.40	0.54
2:B:14:SER:HA	2:B:111:LYS:HB2	1.89	0.53
7:L:301:EPE:H21	3:D:421:GLN:HE22	1.74	0.53
1:H:89:GLU:N	1:H:89:GLU:OE1	2.43	0.52
2:B:4:MET:HG2	2:B:23:CYS:SG	2.50	0.52
2:L:42:GLN:HE22	1:H:39:GLN:HE22	1.57	0.52
1:H:199:THR:HG22	1:H:214:LYS:HG3	1.92	0.52
2:L:216:ASN:OD1	2:L:217:GLU:N	2.43	0.52
1:H:169:HIS:HB2	1:H:185:LEU:HG	1.92	0.52
2:B:56:SER:OG	7:B:301:EPE:O2S	2.25	0.52
3:D:374:GLU:HG3	3:D:412:PRO:HG3	1.92	0.51
3:C:459:ARG:NE	3:C:474:ASP:OD1	2.43	0.51
3:D:476:ASP:O	3:D:478:GLN:N	2.44	0.51
1:H:39:GLN:NE2	9:H:404:HOH:O	2.42	0.50
3:D:451:SER:HB2	3:D:481:LEU:HD11	1.94	0.50
1:H:20:LEU:HD22	1:H:112:THR:HG21	1.93	0.50
1:H:168:VAL:HG22	1:H:186:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:399:ARG:NH2	3:D:430:PRO:O	2.45	0.50
1:A:89:GLU:OE1	1:A:89:GLU:N	2.43	0.50
3:D:338:LEU:HD12	3:D:338:LEU:N	2.27	0.49
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.94	0.49
1:A:37:VAL:HG22	1:A:95:PHE:HB2	1.95	0.49
2:L:41:GLN:HB2	2:L:51:LEU:HD11	1.95	0.49
3:D:435:PHE:CD1	3:D:438:ARG:HG3	2.48	0.49
1:H:160:ASN:HD21	1:H:198:ILE:HD13	1.78	0.49
2:B:122:PHE:HB2	2:B:137:VAL:HG12	1.96	0.48
3:C:431:PRO:HD3	3:C:503:ASN:OD1	2.14	0.48
3:D:369:SER:OG	3:D:370:SER:N	2.47	0.48
1:A:20:LEU:HD22	1:A:112:THR:HG21	1.94	0.48
2:B:4:MET:HE1	2:B:94:HIS:H	1.79	0.47
2:B:194:ASN:ND2	2:B:216[B]:ASN:H	2.12	0.47
2:L:37:MET:O	2:L:55:ALA:N	2.46	0.47
2:L:65:ARG:NH1	2:L:83:GLU:HB2	2.29	0.47
2:B:194:ASN:ND2	2:B:216[A]:ASN:H	2.12	0.47
1:A:37:VAL:HG21	1:A:108:TRP:HZ3	1.79	0.47
1:A:67:LYS:NZ	1:A:85:SER:O	2.29	0.47
2:L:17:GLN:HG3	2:L:18:ARG:H	1.79	0.47
2:B:111:LYS:HA	2:B:144:TYR:OH	2.15	0.47
2:L:197:THR:HG23	2:L:212:SER:HB3	1.97	0.47
2:B:4:MET:HE1	2:B:94:HIS:N	2.30	0.47
2:B:188:ASP:O	2:B:192:ARG:HG3	2.15	0.47
3:C:493:LEU:HD13	3:C:516:LEU:HD21	1.96	0.47
2:L:111:LYS:HA	2:L:144:TYR:OH	2.14	0.47
3:C:427:ILE:HB	5:C:604:GOL:H11	1.97	0.46
1:H:7:SER:HB3	1:H:21:SER:OG	2.15	0.46
1:A:6:GLU:OE2	1:A:111:GLY:N	2.46	0.46
3:D:343:VAL:HA	3:D:369:SER:HB2	1.98	0.46
2:B:33:GLY:O	7:B:301:EPE:H102	2.15	0.46
3:C:374:GLU:HG3	3:C:412:PRO:HG3	1.96	0.46
1:H:11:LEU:HD22	1:H:152:PRO:HG3	1.98	0.46
2:L:43[A]:LYS:NZ	2:L:87:ALA:O	2.47	0.46
1:A:40:ARG:NH1	1:A:91:SER:O	2.48	0.46
2:B:32:SER:HB2	3:C:477:PRO:HD3	1.98	0.46
2:L:65:ARG:HH12	2:L:83:GLU:HB2	1.80	0.46
1:A:155:VAL:HG12	1:A:204:HIS:CD2	2.51	0.45
1:H:98:ARG:HB3	1:H:106[B]:ASP:OD1	2.16	0.45
2:B:14:SER:O	2:B:17:GLN:HG2	2.17	0.45
2:B:194:ASN:ND2	2:B:216[B]:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:SER:OG	1:H:196:GLN:N	2.50	0.45
1:A:155:VAL:HG12	1:A:204:HIS:HD2	1.82	0.45
3:C:346:VAL:HA	3:C:366:GLU:O	2.16	0.45
3:D:337:GLU:C	3:D:338:LEU:HD12	2.37	0.45
3:C:492:LEU:HD12	3:C:492:LEU:HA	1.82	0.45
3:C:380:GLU:HB3	3:C:404:GLY:HA3	1.98	0.45
2:B:129:LEU:O	2:B:187:LYS:NZ	2.45	0.44
2:B:132:GLY:HA2	2:B:187:LYS:HE2	2.00	0.44
3:C:432:TRP:N	3:C:455:SER:O	2.50	0.44
1:H:13:ARG:NH1	1:H:119:ALA:O	2.37	0.44
3:D:442:VAL:HG21	3:D:493:LEU:HD21	1.97	0.44
2:L:37:MET:HE1	2:L:92:CYS:HB2	1.99	0.44
1:A:140:SER:HA	1:A:190:SER:OG	2.18	0.44
1:H:98:ARG:NH2	1:H:106[B]:ASP:OD2	2.48	0.44
1:A:67:LYS:O	1:A:83:LEU:HA	2.18	0.44
1:H:131:PRO:HD3	1:H:143:LEU:HD22	1.99	0.44
2:B:138:CYS:HB2	2:B:152:TRP:CH2	2.52	0.44
2:B:136:VAL:CG1	2:B:183:LEU:HB3	2.48	0.43
3:D:453:GLU:HB2	3:D:481:LEU:HD13	2.00	0.43
3:D:369:SER:HB3	3:D:373:LEU:HD11	1.99	0.43
1:H:53:PRO:HB3	1:H:72:VAL:HG11	2.01	0.43
3:C:371:GLN:HE21	2:L:189:GLU:HB2	1.83	0.43
2:L:37:MET:HG3	2:L:75:PHE:CE1	2.54	0.43
2:L:199:GLU:HB3	2:L:210:VAL:HG12	2.00	0.43
3:C:376:GLN:HG2	3:C:388:ARG:HG2	2.00	0.42
2:L:160:GLN:OE1	2:L:160:GLN:N	2.52	0.42
3:D:491:GLU:O	3:D:495:THR:HG22	2.20	0.42
1:H:210:LYS:HE3	1:H:212:ASP:OD1	2.19	0.42
1:A:169:HIS:ND1	1:A:185:LEU:HD11	2.33	0.42
2:B:37:MET:O	2:B:55:ALA:N	2.48	0.42
1:A:83:LEU:HB3	1:A:86:LEU:HD21	2.01	0.42
3:C:427:ILE:H	5:C:604:GOL:H31	1.84	0.42
2:B:87:ALA:HB2	2:B:110:ILE:HD12	2.01	0.42
3:C:441:TRP:CZ3	3:C:515:GLU:HB3	2.55	0.42
1:A:171:PHE:HE1	1:A:185:LEU:HD23	1.83	0.42
1:A:193:TRP:CE3	1:A:194:PRO:HA	2.54	0.42
2:B:123:PRO:HB3	2:B:213:PHE:CE1	2.55	0.42
3:D:402:GLY:HA2	3:D:425:VAL:HG23	2.02	0.42
3:D:445:ASN:O	3:D:445:ASN:ND2	2.53	0.42
3:C:493:LEU:HD23	3:C:514:LEU:HB3	2.01	0.41
3:D:443:LYS:HE3	3:D:443:LYS:HB2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:MET:HG3	2:L:75:PHE:CD1	2.54	0.41
1:A:98:ARG:NH2	1:A:106:ASP:OD2	2.51	0.41
3:C:338:LEU:HA	3:C:338:LEU:HD23	1.74	0.41
3:C:356:GLN:O	3:C:359:SER:OG	2.29	0.41
2:L:31:ILE:HD13	2:L:96:ARG:CZ	2.51	0.41
1:H:106[B]:ASP:OD1	1:H:107:VAL:N	2.52	0.41
2:B:29:VAL:HA	2:B:96:ARG:HG2	2.03	0.41
3:C:448:LEU:O	3:C:485:ASN:HA	2.20	0.41
3:D:398:LYS:HG3	3:D:400:GLU:OE1	2.21	0.41
1:H:214:LYS:HE2	1:H:214:LYS:HB2	1.91	0.41
2:L:43[A]:LYS:HZ1	2:L:172:SER:HB3	1.86	0.40
2:L:187:LYS:H	2:L:187:LYS:HG3	1.56	0.40
7:L:301:EPE:H21	3:D:421:GLN:NE2	2.34	0.40
1:A:77:SER:OG	5:A:302:GOL:O2	2.26	0.40
1:A:175:LEU:HD13	1:A:180:TYR:CZ	2.57	0.40
3:C:476:ASP:O	3:C:478:GLN:N	2.54	0.40
3:D:489:THR:O	3:D:493:LEU:HD12	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	210/217 (97%)	205 (98%)	5 (2%)	0	100	100
1	H	209/217 (96%)	204 (98%)	5 (2%)	0	100	100
2	B	217/218 (100%)	209 (96%)	7 (3%)	1 (0%)	29	58
2	L	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	C	181/184 (98%)	173 (96%)	6 (3%)	2 (1%)	14	38
3	D	180/184 (98%)	173 (96%)	5 (3%)	2 (1%)	14	38
All	All	1213/1238 (98%)	1173 (97%)	35 (3%)	5 (0%)	34	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	380	GLU
2	B	72	GLY
3	C	380	GLU
3	C	477	PRO
3	D	477	PRO

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	185/187 (99%)	182 (98%)	3 (2%)	62	86
1	H	184/187 (98%)	179 (97%)	5 (3%)	44	75
2	B	192/191 (100%)	188 (98%)	4 (2%)	53	81
2	L	191/191 (100%)	186 (97%)	5 (3%)	46	76
3	C	161/162 (99%)	157 (98%)	4 (2%)	47	77
3	D	160/162 (99%)	153 (96%)	7 (4%)	28	58
All	All	1073/1080 (99%)	1045 (97%)	28 (3%)	46	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	99	SER
1	A	186	MET
2	B	42	GLN
2	B	157	SER
2	B	189	GLU
2	B	195	SER
3	C	381	GLU
3	C	397	LEU
3	C	459	ARG
3	C	481	LEU
2	L	98	LEU

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Mol	Chain	Res	Type
2	L	109	GLU
2	L	147	ASP
2	L	159	ARG
2	L	187	LYS
3	D	338	LEU
3	D	399	ARG
3	D	407	CYS
3	D	420	THR
3	D	466	VAL
3	D	492	LEU
3	D	511	ILE
1	H	55	THR
1	H	99	SER
1	H	195	SER
1	H	199	THR
1	H	216	GLU

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

Mol	Chain	Res	Type
2	B	42	GLN
2	B	194	ASN
2	B	214	ASN
3	C	371	GLN
3	C	376	GLN
3	C	445	ASN
3	C	473	GLN
3	C	475	GLN
3	C	478	GLN
2	L	6	GLN
2	L	42	GLN
2	L	57	ASN
2	L	165	ASN
2	L	194	ASN
3	D	336	GLN
3	D	393	GLN
3	D	421	GLN
3	D	473	GLN
3	D	478	GLN
3	D	485	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

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
7	EPE	B	301	-	15,15,15	0.77	1 (6%)	18,20,20	2.13	6 (33%)
8	NAG	C	602	3	14,14,15	0.40	0	17,19,21	0.45	0
8	NAG	D	602	3	14,14,15	0.41	0	17,19,21	0.59	0
8	NAG	C	601	3	14,14,15	0.31	0	17,19,21	0.58	0
5	GOL	C	604	-	5,5,5	0.84	0	5,5,5	1.00	0
8	NAG	D	601	3	14,14,15	0.96	1 (7%)	17,19,21	0.74	1 (5%)
5	GOL	C	603	-	5,5,5	0.88	0	5,5,5	1.03	0
4	PO4	H	301	-	4,4,4	1.29	0	6,6,6	0.44	0
7	EPE	L	301	-	15,15,15	0.85	1 (6%)	18,20,20	2.16	8 (44%)
4	PO4	A	301	-	4,4,4	1.18	0	6,6,6	0.44	0
5	GOL	A	302	-	5,5,5	1.48	1 (20%)	5,5,5	0.54	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
7	EPE	B	301	-	-	7/9/19/19	0/1/1/1
8	NAG	C	602	3	-	2/6/23/26	0/1/1/1
8	NAG	D	602	3	-	0/6/23/26	0/1/1/1
8	NAG	C	601	3	-	0/6/23/26	0/1/1/1
5	GOL	C	604	-	-	3/4/4/4	-
8	NAG	D	601	3	-	0/6/23/26	0/1/1/1
5	GOL	C	603	-	-	2/4/4/4	-
7	EPE	L	301	-	-	4/9/19/19	0/1/1/1
5	GOL	A	302	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	601	NAG	O5-C1	3.16	1.48	1.43
7	L	301	EPE	C10-S	2.81	1.81	1.77
7	B	301	EPE	C10-S	2.64	1.81	1.77
5	A	302	GOL	C1-C2	2.11	1.60	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	301	EPE	C5-N4-C3	6.10	122.56	108.83
7	L	301	EPE	C6-N1-C2	4.46	118.87	108.83
7	L	301	EPE	C5-N4-C3	4.24	118.38	108.83
7	B	301	EPE	C7-N4-C5	2.75	118.26	111.23
7	B	301	EPE	O3S-S-C10	2.73	110.18	105.77
7	B	301	EPE	C2-C3-N4	2.71	116.20	110.64
7	L	301	EPE	C7-N4-C3	2.60	117.88	111.23
7	B	301	EPE	C7-N4-C3	2.56	117.77	111.23
7	B	301	EPE	O1S-S-C10	2.39	109.80	106.92
7	L	301	EPE	C2-C3-N4	2.34	115.45	110.64
7	L	301	EPE	O1S-S-C10	2.32	109.70	106.92
7	L	301	EPE	O3S-S-C10	2.30	109.48	105.77
7	L	301	EPE	C7-N4-C5	2.26	117.02	111.23
8	D	601	NAG	C1-O5-C5	2.18	115.15	112.19
7	L	301	EPE	C3-C2-N1	2.08	114.92	110.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	GOL	C1-C2-C3-O3
5	C	604	GOL	C1-C2-C3-O3
7	B	301	EPE	S-C10-C9-N1
7	B	301	EPE	C9-C10-S-O2S
7	B	301	EPE	C9-C10-S-O3S
7	L	301	EPE	C9-C10-S-O3S
5	C	603	GOL	O1-C1-C2-C3
5	C	604	GOL	O2-C2-C3-O3
5	A	302	GOL	O2-C2-C3-O3
5	C	603	GOL	O1-C1-C2-O2
7	B	301	EPE	C10-C9-N1-C2
5	A	302	GOL	O1-C1-C2-O2
7	B	301	EPE	C8-C7-N4-C5
7	B	301	EPE	C9-C10-S-O1S
7	L	301	EPE	C9-C10-S-O1S
7	L	301	EPE	C9-C10-S-O2S
7	B	301	EPE	C10-C9-N1-C6
7	L	301	EPE	C10-C9-N1-C6
8	C	602	NAG	C4-C5-C6-O6
8	C	602	NAG	O5-C5-C6-O6
5	A	302	GOL	O1-C1-C2-C3
5	C	604	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	301	EPE	3	0
5	C	604	GOL	3	0
7	L	301	EPE	2	0
5	A	302	GOL	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, 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	212/217 (97%)	0.28	5 (2%)	59	54	39, 60, 108, 129	0
1	H	212/217 (97%)	0.21	5 (2%)	59	54	36, 60, 100, 131	0
2	B	218/218 (100%)	0.20	8 (3%)	41	36	38, 60, 98, 120	0
2	L	217/218 (99%)	0.30	10 (4%)	32	26	38, 61, 101, 125	0
3	C	183/184 (99%)	0.45	10 (5%)	25	19	45, 70, 94, 117	0
3	D	182/184 (98%)	0.46	12 (6%)	18	13	43, 70, 96, 119	0
All	All	1224/1238 (98%)	0.31	50 (4%)	37	32	36, 63, 100, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	338	LEU	5.7
1	A	198	ILE	5.5
3	D	337	GLU	5.5
1	A	186	MET	5.3
1	H	132	VAL	4.9
2	L	213	PHE	4.8
2	L	152	TRP	3.7
2	L	157	SER	3.6
3	D	516	LEU	3.5
3	C	339	LEU	3.5
2	L	197	THR	3.2
2	B	196	TYR	3.2
2	L	205	SER	3.1
1	H	143	LEU	3.0
2	L	185	LEU	2.8
1	A	132	VAL	2.5
3	C	486	VAL	2.5
3	C	400	GLU	2.5
3	D	442	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	196	TYR	2.5
1	A	214	LYS	2.4
3	D	336	GLN	2.4
2	B	82	VAL	2.4
2	B	190	TYR	2.3
3	C	338	LEU	2.3
3	C	373	LEU	2.3
2	L	154	ILE	2.3
1	H	188	VAL	2.3
2	B	21	ILE	2.3
2	L	126	SER	2.2
2	B	191	GLU	2.2
3	D	339	LEU	2.2
3	D	484	LEU	2.2
3	D	511	ILE	2.2
3	C	336	GLN	2.2
2	B	210	VAL	2.2
3	D	441	TRP	2.2
3	C	450	LEU	2.1
2	B	159	ARG	2.1
3	D	514	LEU	2.1
3	D	513	PHE	2.1
1	H	141	VAL	2.1
3	C	340	VAL	2.1
3	C	392	LEU	2.1
1	A	196	GLN	2.0
1	H	211	VAL	2.0
2	B	150	VAL	2.0
2	L	119	VAL	2.0
3	C	337	GLU	2.0
3	D	481	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
5	GOL	A	302	6/6	0.76	0.38	50,57,63,69	0
7	EPE	L	301	15/15	0.79	0.25	43,57,105,106	0
5	GOL	C	604	6/6	0.80	0.53	54,65,68,71	0
6	CL	D	604	1/1	0.84	0.11	67,67,67,67	0
7	EPE	B	301	15/15	0.86	0.19	70,70,75,94	0
5	GOL	C	603	6/6	0.88	0.24	53,59,64,65	0
8	NAG	C	602	14/15	0.88	0.20	66,69,75,76	0
8	NAG	D	601	14/15	0.89	0.17	65,72,83,88	0
8	NAG	C	601	14/15	0.91	0.13	68,74,80,81	0
8	NAG	D	602	14/15	0.91	0.23	61,67,70,74	0
6	CL	A	304	1/1	0.92	0.08	67,67,67,67	0
4	PO4	H	301	5/5	0.93	0.18	76,76,76,76	0
4	PO4	A	301	5/5	0.93	0.17	75,75,75,75	0
6	CL	D	603	1/1	0.95	0.11	77,77,77,77	0
6	CL	A	303	1/1	0.95	0.18	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.