



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2019 – 10:44 AM EST

PDB ID : 6E7K
Title : Structure of the lipoprotein lipase GPIHBP1 complex that mediates plasma triglyceride hydrolysis
Authors : Birrane, G.; Meiyappan, M.
Deposited on : 2018-07-26
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

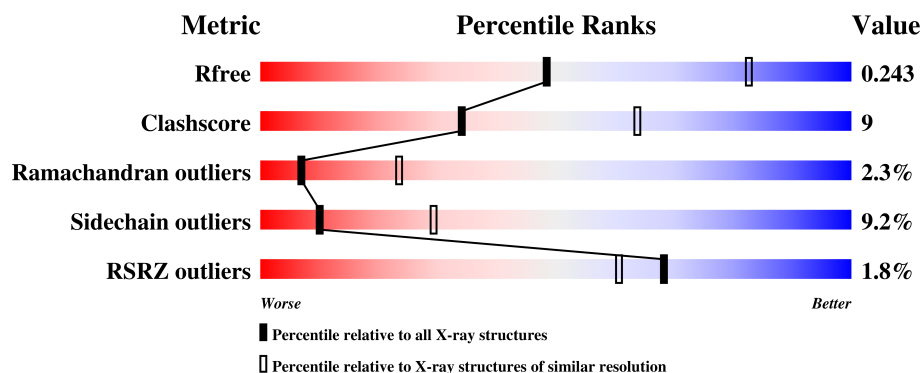
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	448	<div> <div>2%</div> <div>72% 19% 6%</div> </div>
1	B	448	<div> <div>2%</div> <div>74% 16% 6%</div> </div>
2	C	131	<div> <div>34% 21% 8% 37%</div> </div>
2	D	131	<div> <div>2%</div> <div>34% 21% 6% 38%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8045 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3310	2101	568	625	16			
1	B	422	Total	C	N	O	S	0	0	0
			3321	2107	572	626	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	ARG	engineered mutation	UNP P06858
B	324	ALA	ARG	engineered mutation	UNP P06858

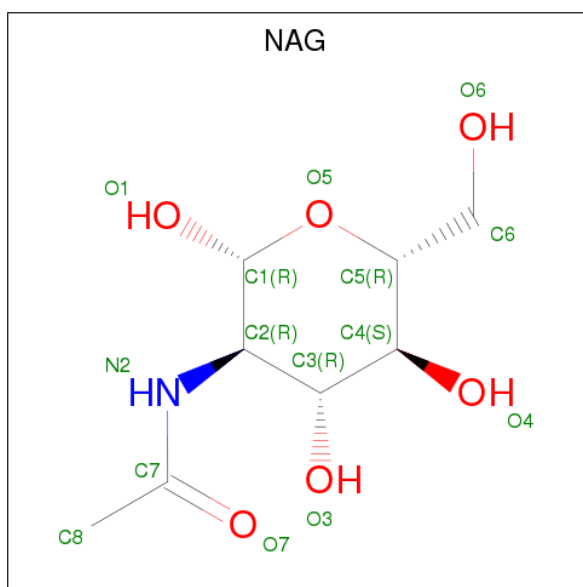
- Molecule 2 is a protein called Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	83	Total	C	N	O	S	0	0	0
			627	376	112	128	11			
2	D	81	Total	C	N	O	S	0	0	0
			615	370	110	124	11			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

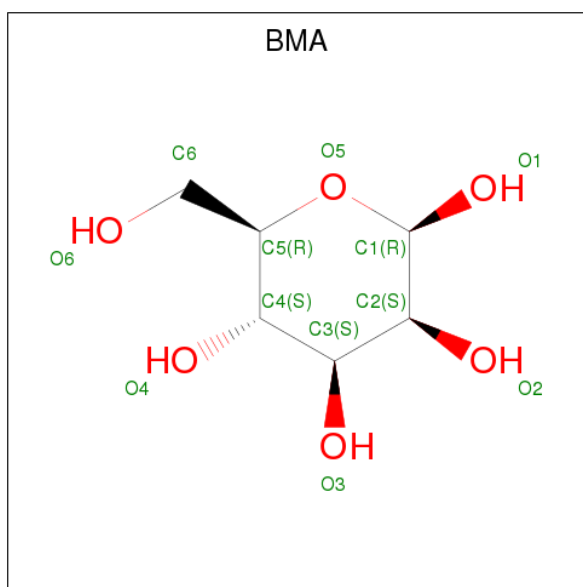
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



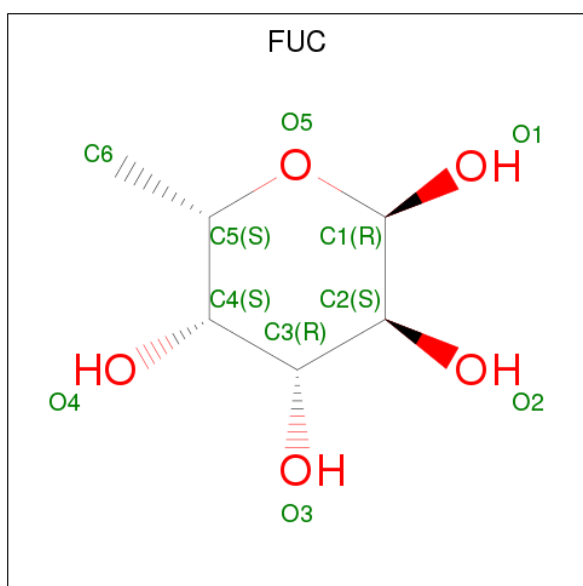
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

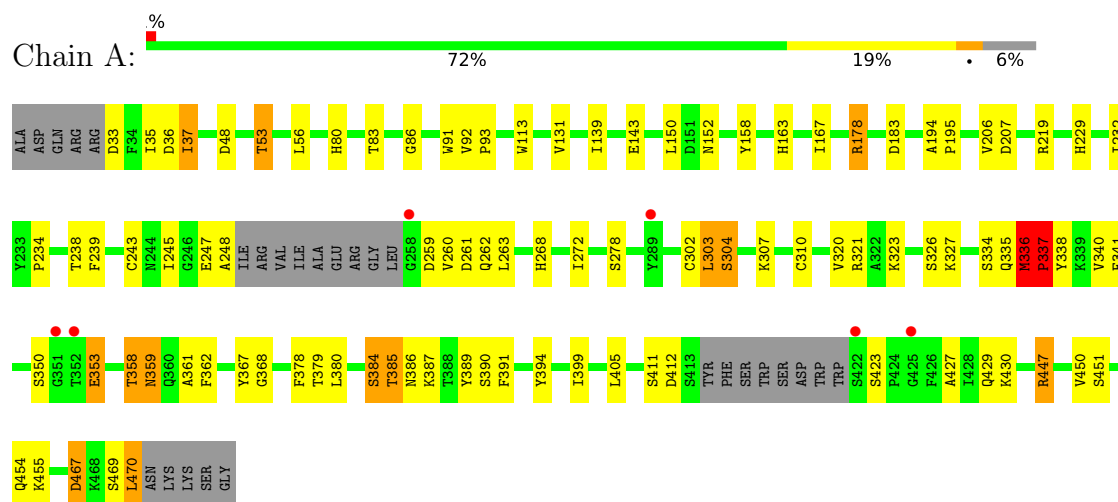
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	B	9	Total 9	O 9	0	0
7	C	1	Total 1	O 1	0	0
7	D	1	Total 1	O 1	0	0

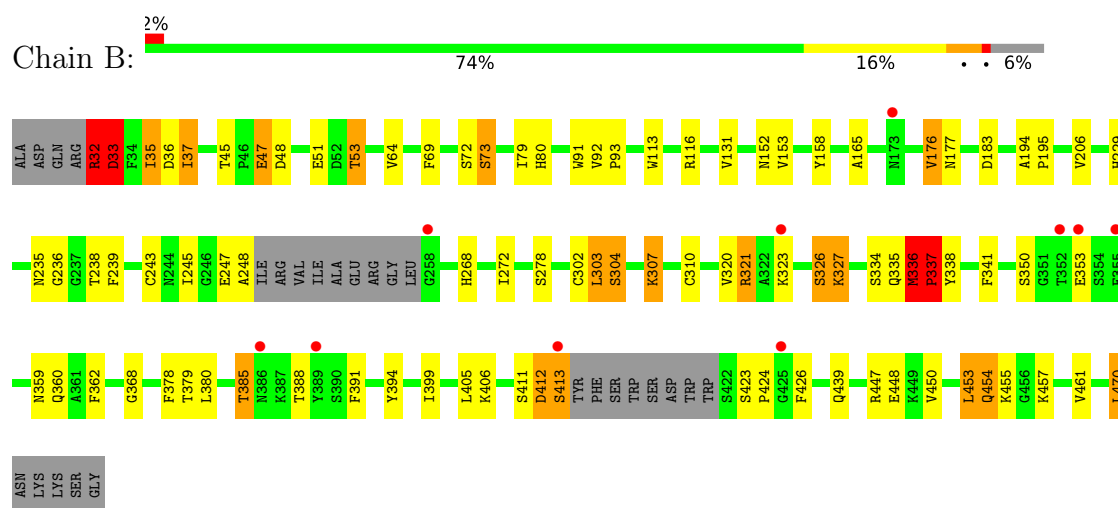
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

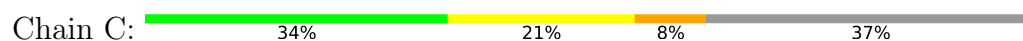
• Molecule 1: Lipoprotein lipase

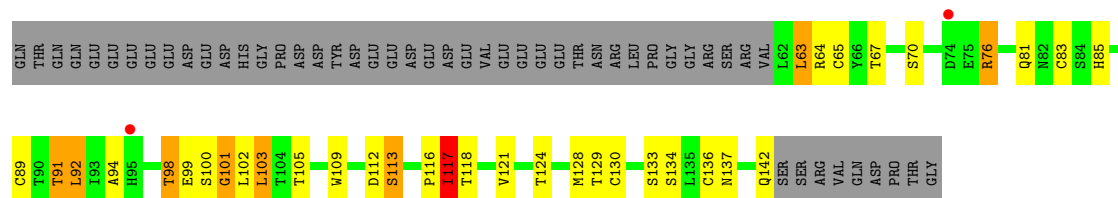


• Molecule 1: Lipoprotein lipase



• Molecule 2: Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.95Å 153.21Å 95.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.80 48.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.41-2.80) 99.3 (48.37-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.195 , 0.235 0.207 , 0.243	Depositor DCC
R_{free} test set	1833 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8045	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, FUC

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	0.53	1/3389 (0.0%)	0.69	1/4585 (0.0%)
1	B	0.54	0/3400	0.71	2/4599 (0.0%)
2	C	0.50	0/638	0.76	0/871
2	D	0.44	0/626	0.79	1/855 (0.1%)
All	All	0.52	1/8053 (0.0%)	0.71	4/10910 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	7
2	C	0	1
2	D	1	3
All	All	1	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	ARG	NE-CZ	6.06	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASN	CB-CA-C	6.62	123.63	110.40
1	B	337	PRO	N-CA-CB	-5.14	96.94	102.60
1	A	337	PRO	N-CA-CB	-5.14	96.95	102.60
2	D	117	ILE	CB-CA-C	5.12	121.85	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	117	ILE	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Sidechain
1	A	302	CYS	Peptide
1	A	33	ASP	Peptide
1	A	336	MET	Peptide
1	A	86	GLY	Peptide
1	B	116	ARG	Sidechain
1	B	236	GLY	Peptide
1	B	302	CYS	Peptide
1	B	32	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	33	ASP	Peptide
1	B	336	MET	Peptide
2	C	64	ARG	Sidechain
2	D	101	GLY	Peptide
2	D	64	ARG	Sidechain
2	D	76	ARG	Sidechain

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	3310	0	3240	54	0
1	B	3321	0	3250	53	0
2	C	627	0	593	30	0
2	D	615	0	583	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	56	0	47	0	0
4	B	42	0	37	0	0
4	C	14	0	13	0	0
5	A	22	0	20	0	0
6	A	10	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	10	0	0
7	A	5	0	0	0	0
7	B	9	0	0	1	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	8045	0	7803	142	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 9.

All (142) 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:359:ASN:O	1:B:380:LEU:O	1.86	0.94
2:C:65:CYS:SG	2:C:89:CYS:HB3	2.13	0.88
1:B:447:ARG:HB3	1:B:447:ARG:HH11	1.38	0.87
1:A:350:SER:OG	1:A:427:ALA:O	1.96	0.82
2:C:91:THR:HG23	2:C:108:THR:HG22	1.62	0.81
1:A:467:ASP:HB2	2:C:109:TRP:HE1	1.46	0.81
1:A:447:ARG:HH12	2:C:96:GLY:H	1.28	0.80
1:A:447:ARG:HH21	2:C:105:THR:HG22	1.45	0.80
1:B:412:ASP:O	1:B:413:SER:HB2	1.84	0.78
1:B:45:THR:OG1	1:B:47:GLU:O	2.04	0.75
2:C:89:CYS:SG	2:C:131:CYS:O	2.45	0.74
2:D:91:THR:HG23	2:D:129:THR:OG1	1.91	0.71
1:B:72:SER:O	1:B:73:SER:HB3	1.93	0.69
1:A:447:ARG:HH12	2:C:96:GLY:N	1.91	0.68
1:A:303:LEU:O	1:A:304:SER:HB3	1.95	0.67
1:B:303:LEU:O	1:B:304:SER:HB3	1.97	0.65
1:B:336:MET:O	1:B:338:TYR:N	2.29	0.65
1:B:35:ILE:O	1:B:35:ILE:HG22	1.95	0.65
1:A:353:GLU:CD	1:A:353:GLU:H	2.01	0.65
1:B:335:GLN:O	1:B:336:MET:O	2.16	0.63
1:A:336:MET:O	1:A:338:TYR:N	2.30	0.63
2:C:89:CYS:HB2	2:C:137:ASN:HB3	1.80	0.63
1:B:411:SER:HA	1:B:455:LYS:HE3	1.79	0.63
1:A:335:GLN:O	1:A:336:MET:O	2.17	0.63
1:A:178:ARG:NH1	1:A:207:ASP:OD1	2.31	0.62
1:A:35:ILE:HG22	1:A:35:ILE:O	2.00	0.61
2:C:89:CYS:SG	2:C:131:CYS:C	2.78	0.61
1:A:48:ASP:OD2	1:A:53:THR:HG21	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:NH2	2:C:105:THR:HG22	2.14	0.61
2:D:67:THR:HG21	2:D:81:GLN:HG3	1.84	0.60
1:B:48:ASP:OD2	1:B:53:THR:HG21	2.02	0.60
1:A:361:ALA:HA	1:A:379:THR:HG22	1.84	0.59
2:C:67:THR:HG21	2:C:81:GLN:HG3	1.83	0.59
2:C:133:SER:O	2:C:136:CYS:SG	2.61	0.59
1:A:467:ASP:HB2	2:C:109:TRP:NE1	2.16	0.58
1:B:439:GLN:O	1:B:470:LEU:HD12	2.04	0.58
2:C:118:THR:HG22	2:C:127:THR:HG23	1.86	0.58
1:B:326:SER:O	1:B:327:LYS:HB2	2.03	0.58
1:A:206:VAL:H	1:A:229:HIS:HD2	1.52	0.57
1:B:206:VAL:H	1:B:229:HIS:HD2	1.52	0.56
2:D:133:SER:O	2:D:136:CYS:SG	2.63	0.56
1:B:177:ASN:ND2	7:B:601:HOH:O	2.35	0.56
1:B:32:ARG:O	1:B:33:ASP:OD1	2.24	0.55
2:D:98:THR:HG23	2:D:101:GLY:N	2.20	0.55
1:B:447:ARG:HH12	2:D:103:LEU:HB3	1.73	0.54
1:B:454:GLN:HG2	1:B:457:LYS:HG3	1.89	0.54
1:A:219:ARG:CZ	1:B:424:PRO:HB3	2.37	0.54
1:B:36:ASP:CG	1:B:37:ILE:N	2.62	0.53
1:B:385:THR:HG22	1:B:426:PHE:HE1	1.74	0.53
2:D:92:LEU:HD22	2:D:128:MET:HG3	1.90	0.53
1:A:469:SER:C	1:A:470:LEU:HG	2.28	0.52
2:D:94:ALA:HB3	2:D:105:THR:CG2	2.40	0.52
2:C:112:ASP:O	2:C:113:SER:C	2.48	0.52
2:D:92:LEU:HD22	2:D:128:MET:CG	2.40	0.52
1:B:153:VAL:HB	1:B:176:VAL:HG22	1.91	0.51
1:A:80:HIS:CE1	1:A:113:TRP:CD1	2.99	0.51
1:B:72:SER:O	1:B:73:SER:CB	2.58	0.51
1:A:384:SER:OG	1:A:389:TYR:OH	2.28	0.50
1:A:247:GLU:O	1:A:248:ALA:C	2.50	0.50
1:A:367:TYR:CZ	2:C:122:GLU:HG3	2.47	0.50
1:A:158:TYR:CG	1:A:272:ILE:HD11	2.46	0.49
1:B:113:TRP:CE3	1:B:131:VAL:HG21	2.48	0.49
1:B:247:GLU:O	1:B:248:ALA:C	2.51	0.49
1:A:447:ARG:NH2	2:C:94:ALA:O	2.46	0.49
1:B:368:GLY:HA3	1:B:399:ILE:HG22	1.94	0.49
1:A:368:GLY:HA3	1:A:399:ILE:HG22	1.95	0.49
1:A:248:ALA:HB1	1:A:262:GLN:OE1	2.13	0.48
2:C:98:THR:OG1	2:C:99:GLU:N	2.47	0.48
1:A:447:ARG:HH21	2:C:105:THR:CG2	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:C	1:A:405:LEU:HD23	2.35	0.48
1:B:80:HIS:CE1	1:B:113:TRP:CD1	3.02	0.48
2:C:78:ASN:O	2:C:78:ASN:OD1	2.32	0.48
1:B:158:TYR:CG	1:B:272:ILE:HD11	2.49	0.47
2:D:65:CYS:SG	2:D:83:CYS:SG	3.11	0.47
2:C:94:ALA:HB3	2:C:105:THR:CG2	2.43	0.47
1:B:405:LEU:HD23	1:B:405:LEU:C	2.34	0.47
2:D:112:ASP:O	2:D:113:SER:C	2.52	0.47
1:B:353:GLU:O	1:B:385:THR:HG21	2.15	0.47
1:A:113:TRP:CE3	1:A:131:VAL:HG21	2.49	0.46
1:A:259:ASP:O	1:A:262:GLN:NE2	2.48	0.46
1:B:35:ILE:O	1:B:35:ILE:CG2	2.61	0.46
1:B:36:ASP:OD2	1:B:37:ILE:N	2.48	0.46
1:B:92:VAL:N	1:B:93:PRO:HD2	2.31	0.46
2:D:67:THR:HG22	2:D:109:TRP:HA	1.96	0.46
1:A:163:HIS:O	1:A:167:ILE:HG13	2.15	0.46
2:C:102:LEU:HD12	2:C:102:LEU:C	2.35	0.46
1:B:320:VAL:HG23	1:B:321:ARG:N	2.31	0.46
2:C:65:CYS:SG	2:C:89:CYS:CB	2.97	0.45
2:C:63:LEU:HD21	2:C:133:SER:C	2.36	0.45
1:A:353:GLU:O	1:A:385:THR:HG21	2.17	0.45
1:B:51:GLU:HB2	1:B:53:THR:HG22	1.99	0.45
2:C:92:LEU:HD22	2:C:128:MET:CG	2.46	0.45
2:D:98:THR:OG1	2:D:99:GLU:N	2.49	0.45
1:A:36:ASP:OD1	1:A:37:ILE:N	2.50	0.45
1:B:91:TRP:CD2	1:B:272:ILE:HD13	2.52	0.44
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.98	0.44
1:B:194:ALA:N	1:B:195:PRO:CD	2.81	0.44
1:A:91:TRP:CD2	1:A:272:ILE:HD13	2.53	0.44
1:A:320:VAL:HG23	1:A:321:ARG:N	2.32	0.44
1:B:307:LYS:CD	1:B:307:LYS:O	2.64	0.44
1:A:194:ALA:N	1:A:195:PRO:CD	2.80	0.44
2:C:67:THR:HG22	2:C:109:TRP:HA	1.99	0.44
1:A:411:SER:HA	1:A:455:LYS:HE3	1.99	0.44
1:A:362:PHE:CE2	1:A:380:LEU:HD12	2.53	0.43
1:B:362:PHE:CE2	1:B:380:LEU:HD12	2.53	0.43
2:D:116:PRO:O	2:D:117:ILE:HD13	2.18	0.43
1:B:206:VAL:N	1:B:229:HIS:HD2	2.16	0.43
2:C:64:ARG:O	2:C:134:SER:HA	2.19	0.43
1:B:239:PHE:CE2	1:B:243:CYS:O	2.72	0.43
2:C:92:LEU:HD22	2:C:128:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:O	1:A:359:ASN:C	2.57	0.42
1:A:378:PHE:CZ	1:A:391:PHE:CZ	3.07	0.42
1:B:453:LEU:O	1:B:454:GLN:CB	2.66	0.42
1:B:406:LYS:HG2	1:B:461:VAL:HG22	2.01	0.42
2:D:89:CYS:HB3	2:D:137:ASN:HB3	2.02	0.42
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.85	0.42
1:A:232:ILE:HG22	1:A:234:PRO:HD3	2.00	0.42
1:A:35:ILE:CG2	1:A:35:ILE:O	2.66	0.42
1:B:378:PHE:CZ	1:B:391:PHE:CZ	3.07	0.42
1:A:219:ARG:NH1	1:B:424:PRO:HB3	2.34	0.42
1:A:36:ASP:CG	1:A:37:ILE:N	2.73	0.42
1:B:64:VAL:HG13	1:B:69:PHE:HB3	2.01	0.42
1:A:139:ILE:CG2	1:A:150:LEU:HD22	2.50	0.42
1:A:183:ASP:OD2	1:A:268:HIS:HD2	2.02	0.42
2:D:117:ILE:CG1	2:D:118:THR:H	2.33	0.42
1:B:341:PHE:O	1:B:394:TYR:HA	2.19	0.42
1:A:341:PHE:O	1:A:394:TYR:HA	2.20	0.41
1:A:367:TYR:HB3	2:C:121:VAL:HG23	2.02	0.41
1:B:183:ASP:OD2	1:B:268:HIS:HD2	2.03	0.41
1:B:307:LYS:O	1:B:307:LYS:HD2	2.21	0.41
2:D:76:ARG:HG2	2:D:142:GLN:OE1	2.20	0.41
1:A:386:ASN:O	1:A:387:LYS:HD2	2.21	0.41
1:A:239:PHE:CE2	1:A:243:CYS:O	2.74	0.41
1:B:79:ILE:HD12	1:B:165:ALA:HB2	2.03	0.41
2:D:117:ILE:HG13	2:D:118:THR:H	1.86	0.41
1:A:353:GLU:CD	1:A:353:GLU:N	2.72	0.41
1:A:260:VAL:HG13	1:A:261:ASP:OD1	2.21	0.41
1:B:158:TYR:CD1	1:B:272:ILE:HD11	2.56	0.40
2:C:106:HIS:CG	2:C:139:PRO:HG3	2.56	0.40
2:D:63:LEU:HD21	2:D:133:SER:CA	2.51	0.40
1:B:36:ASP:CG	1:B:37:ILE:H	2.24	0.40
1:B:336:MET:HB3	1:B:337:PRO:CD	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/448 (93%)	378 (91%)	30 (7%)	7 (2%)	10	32
1	B	416/448 (93%)	371 (89%)	33 (8%)	12 (3%)	5	17
2	C	81/131 (62%)	76 (94%)	3 (4%)	2 (2%)	6	21
2	D	79/131 (60%)	73 (92%)	4 (5%)	2 (2%)	6	21
All	All	991/1158 (86%)	898 (91%)	70 (7%)	23 (2%)	7	23

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	336	MET
1	A	337	PRO
1	A	423	SER
1	B	33	ASP
1	B	37	ILE
1	B	336	MET
1	B	337	PRO
1	B	423	SER
1	B	453	LEU
2	C	121	VAL
2	D	113	SER
1	B	73	SER
2	C	113	SER
2	D	121	VAL
1	A	359	ASN
1	B	454	GLN
1	A	327	LYS
1	B	327	LYS
1	B	360	GLN
1	A	304	SER
1	B	304	SER
1	B	35	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	365/388 (94%)	335 (92%)	30 (8%)	12	35
1	B	366/388 (94%)	342 (93%)	24 (7%)	18	47
2	C	78/122 (64%)	64 (82%)	14 (18%)	2	6
2	D	76/122 (62%)	63 (83%)	13 (17%)	2	6
All	All	885/1020 (87%)	804 (91%)	81 (9%)	10	29

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	56	LEU
1	A	83	THR
1	A	143	GLU
1	A	152	ASN
1	A	238	THR
1	A	245	ILE
1	A	263	LEU
1	A	278	SER
1	A	303	LEU
1	A	307	LYS
1	A	310	CYS
1	A	323	LYS
1	A	326	SER
1	A	334	SER
1	A	337	PRO
1	A	340	VAL
1	A	353	GLU
1	A	358	THR
1	A	384	SER
1	A	385	THR
1	A	390	SER
1	A	412	ASP
1	A	429	GLN
1	A	430	LYS
1	A	450	VAL
1	A	451	SER
1	A	454	GLN

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Mol	Chain	Res	Type
1	A	467	ASP
1	A	470	LEU
1	B	32	ARG
1	B	47	GLU
1	B	53	THR
1	B	152	ASN
1	B	176	VAL
1	B	238	THR
1	B	245	ILE
1	B	278	SER
1	B	303	LEU
1	B	307	LYS
1	B	310	CYS
1	B	323	LYS
1	B	326	SER
1	B	334	SER
1	B	337	PRO
1	B	350	SER
1	B	379	THR
1	B	385	THR
1	B	388	THR
1	B	412	ASP
1	B	413	SER
1	B	448	GLU
1	B	450	VAL
1	B	470	LEU
2	C	63	LEU
2	C	70	SER
2	C	78	ASN
2	C	90	THR
2	C	91	THR
2	C	92	LEU
2	C	97	ASN
2	C	98	THR
2	C	99	GLU
2	C	103	LEU
2	C	119	LYS
2	C	124	THR
2	C	134	SER
2	C	143	SER
2	D	63	LEU
2	D	70	SER

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Mol	Chain	Res	Type
2	D	85	HIS
2	D	91	THR
2	D	92	LEU
2	D	98	THR
2	D	100	SER
2	D	102	LEU
2	D	103	LEU
2	D	117	ILE
2	D	124	THR
2	D	130	CYS
2	D	134	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	224	GLN
1	A	229	HIS
1	A	244	ASN
1	A	268	HIS
1	A	308	ASN
1	A	454	GLN
1	A	466	HIS
1	B	229	HIS
1	B	262	GLN
1	B	268	HIS
1	B	308	ASN
1	B	466	HIS
2	D	95	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 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	NAG	A	502	1,4	14,14,15	0.44	0	17,19,21	1.86	4 (23%)
4	NAG	A	503	5,4	14,14,15	0.57	0	17,19,21	1.61	2 (11%)
5	BMA	A	504	4	11,11,12	0.43	0	15,15,17	0.91	0
4	NAG	A	505	1,4,6	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
6	FUC	A	506	4	9,10,11	0.31	0	13,14,16	1.43	2 (15%)
4	NAG	A	507	5,4	14,14,15	0.54	0	17,19,21	1.75	1 (5%)
5	BMA	A	508	4	11,11,12	0.49	0	15,15,17	1.21	1 (6%)
4	NAG	B	501	1,4,6	14,14,15	0.50	0	17,19,21	1.39	2 (11%)
6	FUC	B	502	4	9,10,11	0.24	0	13,14,16	0.70	0
4	NAG	B	503	4	14,14,15	0.46	0	17,19,21	1.70	2 (11%)
4	NAG	B	504	1	14,14,15	0.63	0	17,19,21	2.25	1 (5%)
4	NAG	C	201	2	14,14,15	0.63	0	17,19,21	1.67	2 (11%)

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	NAG	A	502	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	503	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	504	4	-	0/2/19/22	0/1/1/1
4	NAG	A	505	1,4,6	-	0/6/23/26	0/1/1/1
6	FUC	A	506	4	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	507	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	508	4	-	0/2/19/22	0/1/1/1
4	NAG	B	501	1,4,6	-	0/6/23/26	0/1/1/1
6	FUC	B	502	4	-	0/0/17/20	0/1/1/1
4	NAG	B	503	4	-	0/6/23/26	0/1/1/1
4	NAG	B	504	1	-	0/6/23/26	0/1/1/1
4	NAG	C	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	NAG	O5-C1-C2	-3.51	106.68	111.52
4	B	501	NAG	C1-C2-N2	-3.38	104.71	110.49
4	A	505	NAG	C1-C2-N2	-3.29	104.87	110.49
5	A	508	BMA	O5-C1-C2	-3.15	105.87	110.78
6	A	506	FUC	O5-C1-C2	-3.14	105.89	110.78
4	A	505	NAG	O5-C1-C2	-2.42	108.18	111.52
4	A	503	NAG	C1-O5-C5	-2.41	108.88	112.19
6	A	506	FUC	C2-C3-C4	-2.19	107.07	110.87
4	C	201	NAG	C3-C4-C5	2.55	114.80	110.24
4	A	502	NAG	C1-C2-N2	2.88	115.42	110.49
4	A	502	NAG	C1-O5-C5	3.00	116.31	112.19
4	B	503	NAG	O5-C5-C6	3.13	112.10	107.15
4	B	501	NAG	C4-C3-C2	3.48	116.12	111.02
4	A	503	NAG	C4-C3-C2	3.97	116.83	111.02
4	A	502	NAG	C3-C4-C5	4.42	118.16	110.24
4	C	201	NAG	C1-O5-C5	5.15	119.28	112.19
4	B	503	NAG	C1-O5-C5	5.67	119.98	112.19
4	A	507	NAG	C1-O5-C5	6.56	121.22	112.19
4	B	504	NAG	C1-O5-C5	8.40	123.74	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	421/448 (93%)	0.13	6 (1%) 75 69	69, 91, 132, 149	0
1	B	422/448 (94%)	0.20	10 (2%) 59 49	59, 85, 125, 145	0
2	C	83/131 (63%)	0.06	0 100 100	88, 110, 137, 161	0
2	D	81/131 (61%)	-0.20	2 (2%) 57 47	79, 107, 138, 151	0
All	All	1007/1158 (86%)	0.12	18 (1%) 68 61	59, 91, 133, 161	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	5.0
1	B	258	GLY	3.4
1	A	352	THR	3.2
1	A	422	SER	3.2
1	B	323	LYS	2.8
1	B	173	ASN	2.7
1	A	425	GLY	2.7
1	B	353	GLU	2.6
2	D	95	HIS	2.4
1	A	351	GLY	2.4
1	B	352	THR	2.3
1	B	413	SER	2.2
1	B	389	TYR	2.2
1	A	289	TYR	2.1
1	B	425	GLY	2.1
1	B	386	ASN	2.1
1	B	355	GLU	2.1
2	D	74	ASP	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. 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	B-factors(\AA^2)	Q<0.9
4	NAG	C	201	14/15	0.47	0.38	139,153,159,159	0
5	BMA	A	504	11/12	0.76	0.31	141,152,157,159	0
4	NAG	B	504	14/15	0.76	0.35	107,117,125,127	0
5	BMA	A	508	11/12	0.79	0.29	158,167,169,169	0
4	NAG	B	503	14/15	0.83	0.26	119,130,135,138	0
4	NAG	A	502	14/15	0.86	0.15	105,118,131,142	0
4	NAG	A	503	14/15	0.86	0.29	139,150,155,156	0
4	NAG	B	501	14/15	0.89	0.23	97,112,121,121	0
4	NAG	A	505	14/15	0.90	0.12	93,102,109,113	0
4	NAG	A	507	14/15	0.94	0.21	120,126,136,148	0
6	FUC	A	506	10/11	0.94	0.27	106,113,116,119	0
6	FUC	B	502	10/11	0.95	0.15	112,113,116,116	0
3	CA	A	501	1/1	0.96	0.09	98,98,98,98	0
3	CA	B	505	1/1	0.97	0.08	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.