



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:49 AM BST

PDB ID : 6OAZ
Title : Apo Structure of WT Lipoprotein Lipase in Complex with GPIHBP1 Mutant N78D N82D produced in HEK293-F cells
Authors : Arora, R.; Horton, P.A.; Benson, T.E.; Romanowski, M.J.
Deposited on : 2019-03-19
Resolution : 3.04 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

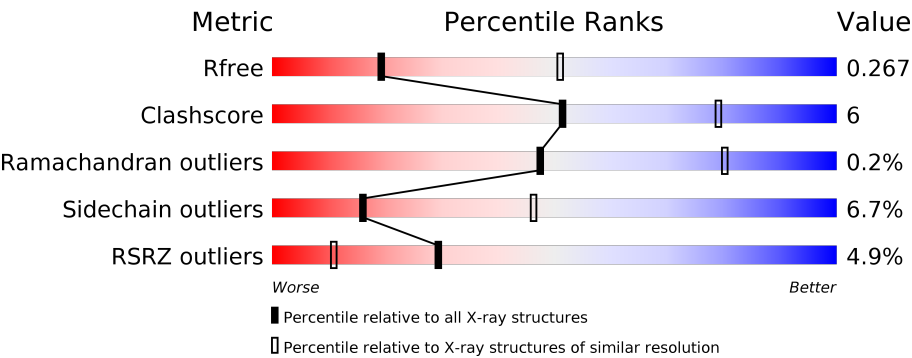
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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 $\leq 5\%$. 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><div></div><div>75%</div><div>17%</div><div>7%</div></div></div>
1	B	448	<div><div>4%</div><div><div></div><div>78%</div><div>15%</div><div>7%</div></div></div>
1	C	448	<div><div>2%</div><div><div></div><div>78%</div><div>15%</div><div>7%</div></div></div>
1	D	448	<div><div>2%</div><div><div></div><div>77%</div><div>15%</div><div>7%</div></div></div>
2	E	131	<div><div>5%</div><div><div></div><div>44%</div><div>18%</div><div>37%</div></div></div>
2	F	131	<div><div>20%</div><div><div></div><div>42%</div><div>18%</div><div>40%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	131	<div><div><div></div><div></div><div></div><div></div></div><div>10%42%18%•38%</div></div>
2	H	131	<div><div><div></div><div></div><div></div><div></div></div><div>3%41%18%•39%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15843 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	416	Total	C	N	O	S	0	0	0
			3307	2104	575	612	16			
1	B	416	Total	C	N	O	S	0	0	0
			3307	2104	575	612	16			
1	C	416	Total	C	N	O	S	0	0	0
			3307	2104	575	612	16			
1	D	416	Total	C	N	O	S	0	0	0
			3307	2104	575	612	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	83	Total	C	N	O	S	0	0	0
			628	378	110	129	11			
2	F	79	Total	C	N	O	S	0	0	0
			594	355	103	125	11			
2	G	81	Total	C	N	O	S	0	0	0
			613	367	108	127	11			
2	H	80	Total	C	N	O	S	0	0	0
			607	364	107	125	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ASP	ASN	engineered mutation	UNP Q8IV16
E	82	ASP	ASN	engineered mutation	UNP Q8IV16
F	78	ASP	ASN	engineered mutation	UNP Q8IV16
F	82	ASP	ASN	engineered mutation	UNP Q8IV16
G	78	ASP	ASN	engineered mutation	UNP Q8IV16
G	82	ASP	ASN	engineered mutation	UNP Q8IV16
H	78	ASP	ASN	engineered mutation	UNP Q8IV16
H	82	ASP	ASN	engineered mutation	UNP Q8IV16

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		
5	D	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		

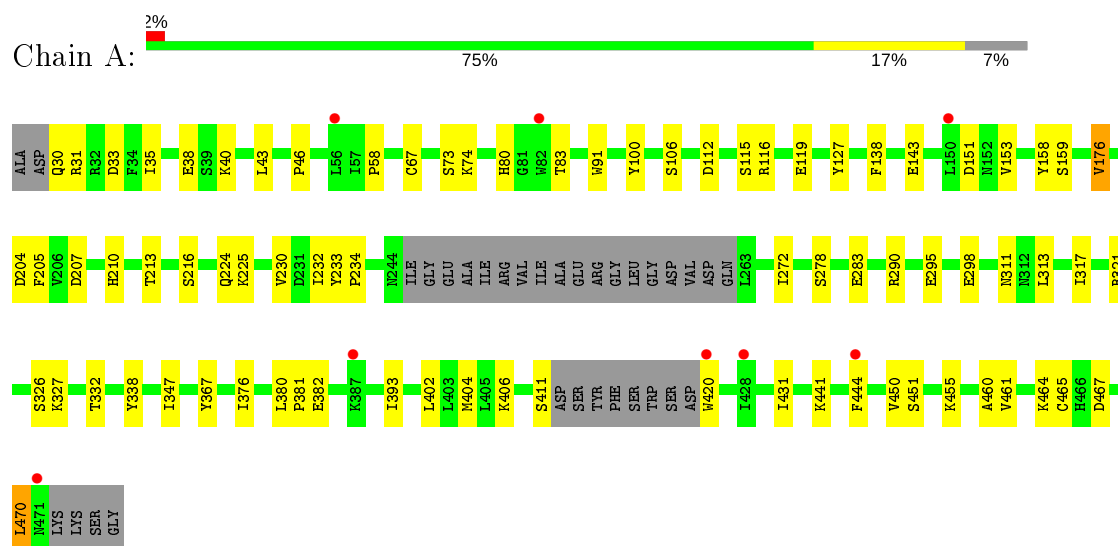
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	B	4	Total 4	O 4	0	0
6	C	5	Total 5	O 5	0	0
6	D	6	Total 6	O 6	0	0

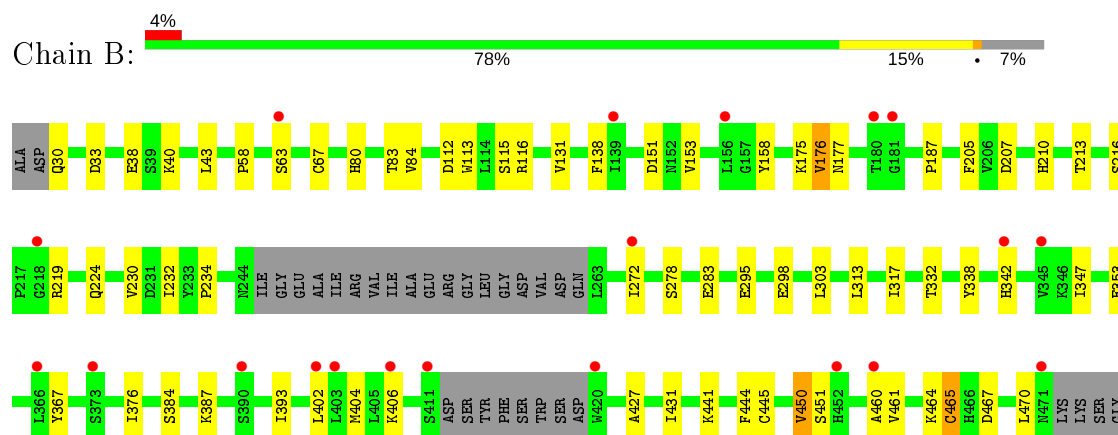
3 Residue-property plots [i](#)

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.

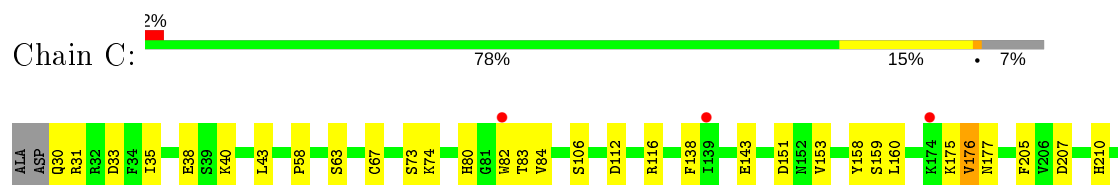
• Molecule 1: Lipoprotein lipase

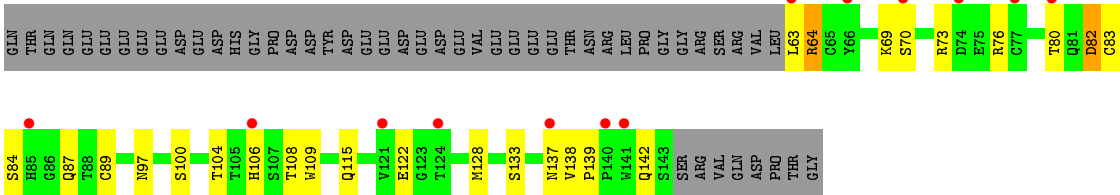


• Molecule 1: Lipoprotein lipase

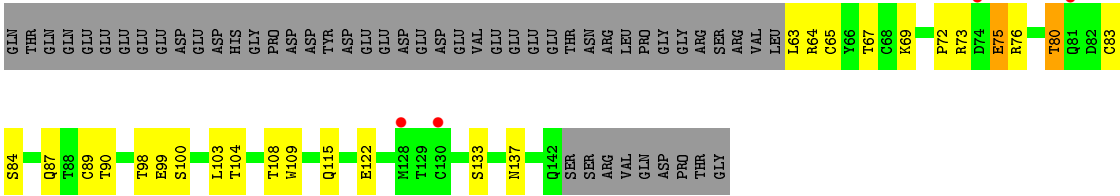


• Molecule 1: Lipoprotein lipase





● 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	157.00 Å 191.94 Å 96.06 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.52 – 3.04 121.52 – 3.04	Depositor EDS
% Data completeness (in resolution range)	97.0 (121.52-3.04) 97.1 (121.52-3.04)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.01 Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.203 , 0.245 0.223 , 0.267	Depositor DCC
R_{free} test set	2738 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15843	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6810e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/3390	0.71	0/4586
1	B	0.51	0/3390	0.69	0/4586
1	C	0.51	0/3390	0.69	0/4586
1	D	0.53	0/3390	0.70	0/4586
2	E	0.52	0/639	0.77	1/873 (0.1%)
2	F	0.54	0/605	0.72	0/827
2	G	0.52	0/624	0.72	1/852 (0.1%)
2	H	0.52	0/618	0.73	0/844
All	All	0.52	0/16046	0.70	2/21740 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	70	SER	N-CA-C	6.13	127.55	111.00
2	G	70	SER	N-CA-C	5.38	125.52	111.00

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	3307	0	3243	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3307	0	3243	33	0
1	C	3307	0	3243	33	0
1	D	3307	0	3243	38	0
2	E	628	0	593	13	0
2	F	594	0	549	11	0
2	G	613	0	573	13	0
2	H	607	0	568	17	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	8	0	12	2	0
4	B	8	0	12	3	0
4	C	8	0	12	3	0
4	D	8	0	12	6	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	6	0	0	0	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
6	D	6	0	0	0	0
All	All	15843	0	15407	176	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 (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:HIS:HB2	4:D:503:EDO:H21	1.52	0.91
1:D:441:LYS:HG3	1:D:470:LEU:HD11	1.56	0.88
1:C:441:LYS:HG3	1:C:470:LEU:HD11	1.62	0.81
1:B:80:HIS:HB2	4:B:503:EDO:H12	1.63	0.80
1:C:467:ASP:HB2	2:G:109:TRP:HE1	1.48	0.79
1:B:441:LYS:HG3	1:B:470:LEU:HD11	1.64	0.79
1:D:467:ASP:HB2	2:H:109:TRP:HE1	1.47	0.79
1:C:402:LEU:HB3	1:C:444:PHE:HZ	1.55	0.72
1:B:402:LEU:HB3	1:B:444:PHE:HZ	1.56	0.70
1:D:80:HIS:HB2	4:D:503:EDO:C2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASP:HB2	2:E:109:TRP:HE1	1.57	0.69
1:A:402:LEU:HB3	1:A:444:PHE:HZ	1.57	0.69
1:D:402:LEU:HB3	1:D:444:PHE:HZ	1.57	0.68
1:B:115:SER:H	4:B:504:EDO:H12	1.61	0.66
1:D:404:MET:HE1	2:H:122:GLU:HB2	1.77	0.65
1:B:467:ASP:HB2	2:F:109:TRP:HE1	1.64	0.63
2:E:61:VAL:HA	2:H:80:THR:O	1.99	0.63
1:C:307:LYS:HD2	1:C:309:ARG:NH1	2.14	0.62
1:B:445:CYS:SG	2:F:70:SER:HB2	2.40	0.61
1:A:404:MET:HE1	2:E:122:GLU:HB2	1.81	0.61
1:A:116:ARG:HD3	1:A:127:TYR:CD1	2.35	0.60
2:E:92:LEU:HD21	2:E:126:VAL:HG13	1.84	0.60
2:G:108:THR:HB	2:G:137:ASN:ND2	2.17	0.59
1:C:467:ASP:HB2	2:G:109:TRP:NE1	2.15	0.59
1:A:153:VAL:HB	1:A:176:VAL:HG12	1.85	0.59
2:G:139:PRO:HG2	2:G:142:GLN:HB2	1.84	0.59
1:C:404:MET:HE1	2:G:122:GLU:HB2	1.85	0.58
1:B:213:THR:HB	1:B:224:GLN:HG2	1.84	0.58
2:H:63:LEU:HD23	2:H:83:CYS:SG	2.43	0.58
1:C:153:VAL:HB	1:C:176:VAL:HG12	1.86	0.57
1:D:153:VAL:HB	1:D:176:VAL:HG12	1.86	0.57
1:B:153:VAL:HB	1:B:176:VAL:HG12	1.87	0.57
1:C:406:LYS:HG2	1:C:461:VAL:HG22	1.86	0.57
2:F:90:THR:O	2:F:108:THR:HA	2.05	0.56
1:A:213:THR:HB	1:A:224:GLN:HG2	1.88	0.56
1:D:158:TYR:CD1	1:D:272:ILE:HD11	2.41	0.56
1:D:384:SER:HB3	1:D:387:LYS:HD2	1.87	0.55
2:H:89:CYS:HB3	2:H:137:ASN:HB3	1.87	0.55
1:B:465:CYS:HB2	2:F:69:LYS:HG2	1.89	0.55
1:A:441:LYS:HG3	1:A:470:LEU:HD11	1.88	0.55
1:B:406:LYS:HG2	1:B:461:VAL:HG22	1.89	0.54
1:D:115:SER:CB	4:D:504:EDO:H22	2.37	0.54
1:B:347:ILE:HG12	1:B:431:ILE:HG12	1.90	0.54
2:E:65:CYS:SG	2:E:83:CYS:SG	3.06	0.54
1:A:406:LYS:HG2	1:A:461:VAL:HG22	1.90	0.53
1:D:404:MET:CE	2:H:122:GLU:HB2	2.39	0.53
2:H:67:THR:HG22	2:H:109:TRP:HA	1.90	0.53
1:D:80:HIS:HB2	4:D:503:EDO:C1	2.39	0.53
2:E:133:SER:HB2	2:E:136:CYS:HB3	1.90	0.53
1:B:80:HIS:HB2	4:B:503:EDO:C1	2.37	0.53
1:A:115:SER:HB3	4:A:504:EDO:H21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:HB2	4:A:503:EDO:H12	1.91	0.52
1:A:347:ILE:HG12	1:A:431:ILE:HG12	1.92	0.52
1:C:307:LYS:HD2	1:C:309:ARG:HH12	1.75	0.52
1:A:411:SER:HA	1:A:455:LYS:HE3	1.91	0.52
1:A:467:ASP:HB2	2:E:109:TRP:NE1	2.23	0.52
2:G:106:HIS:CE1	2:G:142:GLN:HE22	2.28	0.51
1:A:233:TYR:CE1	1:A:327:LYS:HD2	2.45	0.51
1:C:347:ILE:HG12	1:C:431:ILE:HG12	1.91	0.51
1:D:406:LYS:HG2	1:D:461:VAL:HG22	1.92	0.51
2:F:118:THR:HB	2:F:127:THR:HG23	1.91	0.51
1:D:467:ASP:HB2	2:H:109:TRP:NE1	2.21	0.50
1:D:347:ILE:HG12	1:D:431:ILE:HG12	1.91	0.50
1:C:82:TRP:HB2	1:C:160:LEU:HD12	1.94	0.50
1:D:58:PRO:HG3	1:D:138:PHE:HD1	1.77	0.50
1:A:58:PRO:HG3	1:A:138:PHE:HD1	1.78	0.49
1:A:232:ILE:HG21	1:A:313:LEU:HD12	1.95	0.49
1:A:205:PHE:CE2	1:A:207:ASP:HB3	2.48	0.49
1:B:158:TYR:CD1	1:B:272:ILE:HD11	2.47	0.49
1:A:38:GLU:HB3	1:A:116:ARG:HH21	1.77	0.49
1:C:451:SER:HB3	1:C:460:ALA:HB1	1.95	0.48
1:A:204:ASP:HA	1:A:321:ARG:HH11	1.79	0.48
1:B:40:LYS:HB2	1:B:112:ASP:HB3	1.95	0.48
1:C:213:THR:HB	1:C:224:GLN:HG2	1.94	0.48
1:C:332:THR:HB	1:C:338:TYR:HB3	1.96	0.48
1:D:213:THR:HB	1:D:224:GLN:HG2	1.95	0.48
1:D:232:ILE:HG21	1:D:313:LEU:HD12	1.95	0.48
1:D:205:PHE:CE2	1:D:207:ASP:HB3	2.48	0.48
2:F:98:THR:HG21	2:F:103:LEU:HD23	1.96	0.48
1:C:205:PHE:CE2	1:C:207:ASP:HB3	2.48	0.48
1:C:465:CYS:HB2	2:G:69:LYS:HG2	1.96	0.48
1:D:332:THR:HB	1:D:338:TYR:HB3	1.96	0.48
1:C:38:GLU:HB3	1:C:116:ARG:HH11	1.78	0.48
1:A:290:ARG:HG3	1:A:326:SER:HB2	1.95	0.47
1:B:332:THR:HB	1:B:338:TYR:HB3	1.96	0.47
2:F:83:CYS:HB3	2:F:87:GLN:HB2	1.96	0.47
1:D:116:ARG:HD3	1:D:127:TYR:CD1	2.49	0.47
1:B:205:PHE:CE2	1:B:207:ASP:HB3	2.49	0.47
1:B:467:ASP:HB2	2:F:109:TRP:NE1	2.27	0.47
1:C:232:ILE:HG21	1:C:313:LEU:HD12	1.96	0.47
2:F:73:ARG:HB2	2:F:104:THR:HB	1.96	0.47
1:D:91:TRP:CD2	1:D:272:ILE:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:SER:O	2:E:136:CYS:SG	2.73	0.47
2:H:108:THR:HB	2:H:137:ASN:ND2	2.29	0.47
1:B:376:ILE:HG21	1:B:393:ILE:HG23	1.96	0.46
1:B:43:LEU:HD23	1:B:67:CYS:HB3	1.97	0.46
2:H:98:THR:HG21	2:H:103:LEU:HD23	1.97	0.46
1:C:376:ILE:HG21	1:C:393:ILE:HG23	1.96	0.46
2:H:72:PRO:HG2	2:H:75:GLU:HB2	1.96	0.46
2:H:73:ARG:HB2	2:H:104:THR:HB	1.97	0.46
2:H:65:CYS:SG	2:H:83:CYS:SG	3.13	0.46
1:C:38:GLU:HB3	1:C:116:ARG:NH1	2.30	0.46
1:B:451:SER:HB3	1:B:460:ALA:HB1	1.97	0.46
2:E:94:ALA:O	2:E:104:THR:HA	2.16	0.46
1:C:40:LYS:HB2	1:C:112:ASP:HB3	1.97	0.46
1:C:80:HIS:HB2	4:C:503:EDO:H12	1.97	0.46
1:D:210:HIS:O	1:D:234:PRO:HD2	2.16	0.46
1:C:58:PRO:HG3	1:C:138:PHE:HD1	1.80	0.46
1:D:115:SER:HB3	4:D:504:EDO:H22	1.97	0.46
1:D:159:SER:HB2	1:D:268:HIS:NE2	2.30	0.45
1:A:332:THR:HB	1:A:338:TYR:HB3	1.98	0.45
1:A:451:SER:HB3	1:A:460:ALA:HB1	1.97	0.45
1:B:232:ILE:HG21	1:B:313:LEU:HD12	1.97	0.45
1:B:230:VAL:HG11	1:B:317:ILE:HD11	1.99	0.45
1:D:376:ILE:HG21	1:D:393:ILE:HG23	1.98	0.45
1:A:91:TRP:CD2	1:A:272:ILE:HD13	2.51	0.45
1:A:376:ILE:HG21	1:A:393:ILE:HG23	1.97	0.45
1:A:40:LYS:HB2	1:A:112:ASP:HB3	1.98	0.45
1:C:210:HIS:O	1:C:234:PRO:HD2	2.17	0.45
2:H:83:CYS:HB3	2:H:87:GLN:HB2	1.98	0.45
1:A:230:VAL:HG11	1:A:317:ILE:HD11	1.99	0.45
1:A:210:HIS:O	1:A:234:PRO:HD2	2.16	0.44
1:B:210:HIS:O	1:B:234:PRO:HD2	2.18	0.44
1:C:402:LEU:HB3	1:C:444:PHE:CZ	2.45	0.44
1:C:80:HIS:HB2	4:C:503:EDO:H21	1.99	0.44
1:D:367:TYR:HB2	1:D:404:MET:HB3	1.99	0.44
2:G:63:LEU:HD21	2:G:89:CYS:SG	2.58	0.44
1:B:58:PRO:HG3	1:B:138:PHE:HD1	1.82	0.44
2:G:83:CYS:HB3	2:G:87:GLN:HB2	2.00	0.44
1:C:43:LEU:HD23	1:C:67:CYS:HB3	2.00	0.44
1:D:40:LYS:HB2	1:D:112:ASP:HB3	1.99	0.43
1:D:43:LEU:HD23	1:D:67:CYS:HB3	2.00	0.43
1:D:143:GLU:O	1:D:147:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:CYS:HB2	2:H:69:LYS:HG2	2.00	0.43
2:G:73:ARG:HB2	2:G:104:THR:HB	2.00	0.43
1:D:39:SER:HA	4:D:504:EDO:H12	2.01	0.43
2:E:141:TRP:CD1	2:E:142:GLN:HG3	2.54	0.43
1:B:367:TYR:HB2	1:B:404:MET:HB3	1.99	0.43
1:C:367:TYR:HB2	1:C:404:MET:HB3	2.00	0.43
1:D:230:VAL:HG11	1:D:317:ILE:HD11	2.01	0.43
2:G:108:THR:HB	2:G:137:ASN:HD22	1.82	0.43
2:H:90:THR:O	2:H:108:THR:HA	2.19	0.43
1:A:158:TYR:CD1	1:A:272:ILE:HD11	2.54	0.42
1:C:35:ILE:HG13	1:C:35:ILE:H	1.73	0.42
1:C:73:SER:HB3	1:C:106:SER:HA	2.00	0.42
1:A:38:GLU:HB3	1:A:116:ARG:NH2	2.33	0.42
1:A:43:LEU:HD23	1:A:67:CYS:HB3	2.01	0.42
1:D:73:SER:HB3	1:D:106:SER:HA	2.00	0.42
1:D:151:ASP:O	1:D:177:ASN:HB2	2.20	0.42
1:A:367:TYR:HB2	1:A:404:MET:HB3	2.01	0.42
1:D:303:LEU:HD11	1:D:342:HIS:HB3	2.01	0.42
2:G:64:ARG:HH21	2:G:80:THR:HG23	1.84	0.42
1:A:73:SER:HB3	1:A:106:SER:HA	2.02	0.41
1:B:384:SER:HB2	1:B:387:LYS:HD2	2.02	0.41
1:B:404:MET:HE2	2:F:121:VAL:HG22	2.01	0.41
1:B:113:TRP:CE3	1:B:131:VAL:HG21	2.55	0.41
1:B:303:LEU:HD11	1:B:342:HIS:HB3	2.02	0.41
2:E:73:ARG:HB2	2:E:104:THR:HB	2.02	0.41
2:F:67:THR:HA	2:F:108:THR:O	2.21	0.41
1:C:230:VAL:HG11	1:C:317:ILE:HD11	2.03	0.41
1:A:233:TYR:CZ	1:A:327:LYS:HD2	2.56	0.41
1:B:219:ARG:HH11	1:B:219:ARG:HG2	1.86	0.41
2:E:111:THR:HG23	2:E:114:CYS:HB2	2.03	0.41
1:D:158:TYR:O	1:D:159:SER:C	2.59	0.41
1:A:380:LEU:HA	1:A:381:PRO:HD2	1.90	0.41
1:C:158:TYR:CD1	1:C:272:ILE:HD11	2.55	0.41
1:D:38:GLU:HB3	1:D:116:ARG:NH2	2.36	0.41
1:A:46:PRO:HG3	1:A:100:TYR:CD1	2.56	0.41
2:E:83:CYS:HB3	2:E:87:GLN:HB2	2.03	0.41
1:A:35:ILE:H	1:A:35:ILE:HG13	1.72	0.40
1:B:38:GLU:HB3	1:B:116:ARG:NH1	2.36	0.40
2:G:64:ARG:HH11	2:G:82:ASP:HB2	1.86	0.40
1:A:420:TRP:HE3	1:B:187:PRO:HG2	1.86	0.40
1:B:427:ALA:HB1	1:B:450:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:HB	4:C:503:EDO:H22	2.03	0.40
2:H:90:THR:HG22	2:H:109:TRP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/448 (92%)	390 (95%)	20 (5%)	0	100	100
1	B	410/448 (92%)	392 (96%)	17 (4%)	1 (0%)	47	80
1	C	410/448 (92%)	394 (96%)	15 (4%)	1 (0%)	47	80
1	D	410/448 (92%)	390 (95%)	19 (5%)	1 (0%)	47	80
2	E	81/131 (62%)	76 (94%)	4 (5%)	1 (1%)	13	44
2	F	77/131 (59%)	71 (92%)	6 (8%)	0	100	100
2	G	79/131 (60%)	74 (94%)	5 (6%)	0	100	100
2	H	78/131 (60%)	77 (99%)	1 (1%)	0	100	100
All	All	1955/2316 (84%)	1864 (95%)	87 (4%)	4 (0%)	47	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	ASN
2	E	70	SER
1	C	177	ASN
1	D	177	ASN

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	364/389 (94%)	342 (94%)	22 (6%)	19	51
1	B	364/389 (94%)	347 (95%)	17 (5%)	26	61
1	C	364/389 (94%)	343 (94%)	21 (6%)	20	52
1	D	364/389 (94%)	343 (94%)	21 (6%)	20	52
2	E	78/122 (64%)	70 (90%)	8 (10%)	7	26
2	F	74/122 (61%)	64 (86%)	10 (14%)	4	16
2	G	76/122 (62%)	66 (87%)	10 (13%)	4	16
2	H	75/122 (62%)	66 (88%)	9 (12%)	5	20
All	All	1759/2044 (86%)	1641 (93%)	118 (7%)	16	46

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	ARG
1	A	33	ASP
1	A	74	LYS
1	A	83	THR
1	A	119	GLU
1	A	143	GLU
1	A	151	ASP
1	A	159	SER
1	A	176	VAL
1	A	216	SER
1	A	225	LYS
1	A	278	SER
1	A	283	GLU
1	A	295	GLU
1	A	298	GLU
1	A	311	ASN
1	A	382	GLU
1	A	450	VAL

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Mol	Chain	Res	Type
1	A	464	LYS
1	A	465	CYS
1	A	470	LEU
1	B	30	GLN
1	B	33	ASP
1	B	63	SER
1	B	83	THR
1	B	84	VAL
1	B	151	ASP
1	B	175	LYS
1	B	176	VAL
1	B	216	SER
1	B	278	SER
1	B	283	GLU
1	B	295	GLU
1	B	298	GLU
1	B	353	GLU
1	B	450	VAL
1	B	464	LYS
1	B	465	CYS
1	C	30	GLN
1	C	31	ARG
1	C	33	ASP
1	C	63	SER
1	C	74	LYS
1	C	84	VAL
1	C	143	GLU
1	C	151	ASP
1	C	159	SER
1	C	175	LYS
1	C	176	VAL
1	C	216	SER
1	C	278	SER
1	C	283	GLU
1	C	295	GLU
1	C	298	GLU
1	C	339	LYS
1	C	353	GLU
1	C	451	SER
1	C	464	LYS
1	C	465	CYS
1	D	30	GLN

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Mol	Chain	Res	Type
1	D	33	ASP
1	D	63	SER
1	D	74	LYS
1	D	84	VAL
1	D	119	GLU
1	D	143	GLU
1	D	151	ASP
1	D	175	LYS
1	D	176	VAL
1	D	216	SER
1	D	225	LYS
1	D	267	SER
1	D	278	SER
1	D	283	GLU
1	D	295	GLU
1	D	298	GLU
1	D	440	LYS
1	D	451	SER
1	D	464	LYS
1	D	465	CYS
2	E	76	ARG
2	E	84	SER
2	E	88	THR
2	E	97	ASN
2	E	99	GLU
2	E	100	SER
2	E	115	GLN
2	E	133	SER
2	F	70	SER
2	F	75	GLU
2	F	81	GLN
2	F	82	ASP
2	F	84	SER
2	F	100	SER
2	F	115	GLN
2	F	128	MET
2	F	133	SER
2	F	138	VAL
2	G	64	ARG
2	G	76	ARG
2	G	82	ASP
2	G	84	SER

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Mol	Chain	Res	Type
2	G	97	ASN
2	G	100	SER
2	G	115	GLN
2	G	128	MET
2	G	133	SER
2	G	138	VAL
2	H	64	ARG
2	H	75	GLU
2	H	76	ARG
2	H	80	THR
2	H	84	SER
2	H	99	GLU
2	H	100	SER
2	H	115	GLN
2	H	133	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	GLN
1	D	439	GLN
2	E	142	GLN
2	G	106	HIS
2	H	106	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	EDO	D	503	-	3,3,3	1.20	0	2,2,2	0.23	0
4	EDO	A	504	-	3,3,3	0.99	0	2,2,2	0.42	0
3	NAG	A	502	1	14,14,15	0.41	0	17,19,21	1.05	1 (5%)
4	EDO	B	504	-	3,3,3	1.11	0	2,2,2	0.39	0
4	EDO	C	504	-	3,3,3	1.00	0	2,2,2	0.32	0
3	NAG	C	501	1	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
4	EDO	D	504	-	3,3,3	1.23	0	2,2,2	0.46	0
3	NAG	A	501	1	14,14,15	0.31	0	17,19,21	0.81	1 (5%)
3	NAG	D	502	1	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
3	NAG	B	501	1	14,14,15	0.30	0	17,19,21	0.74	1 (5%)
4	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.45	0
3	NAG	D	501	1	14,14,15	0.31	0	17,19,21	0.79	1 (5%)
4	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.67	0
3	NAG	B	502	1	14,14,15	0.42	0	17,19,21	0.98	1 (5%)
4	EDO	B	503	-	3,3,3	0.55	0	2,2,2	0.62	0
3	NAG	C	502	1	14,14,15	0.47	0	17,19,21	1.04	1 (5%)

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	EDO	D	503	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1
4	EDO	D	504	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	EDO	A	503	-	-	1/1/1/1	-
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	EDO	C	503	-	-	1/1/1/1	-
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
4	EDO	B	503	-	-	1/1/1/1	-
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C1-O5-C5	3.92	117.51	112.19
3	C	502	NAG	C1-O5-C5	3.63	117.11	112.19
3	B	502	NAG	C1-O5-C5	3.61	117.09	112.19
3	D	502	NAG	C1-O5-C5	3.26	116.61	112.19
3	A	501	NAG	C1-O5-C5	3.00	116.25	112.19
3	D	501	NAG	C1-O5-C5	2.65	115.78	112.19
3	C	501	NAG	C1-O5-C5	2.57	115.67	112.19
3	B	501	NAG	C1-O5-C5	2.55	115.65	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	A	503	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	EDO	3	0
4	A	504	EDO	1	0
4	B	504	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	EDO	3	0
4	A	503	EDO	1	0
4	C	503	EDO	3	0
4	B	503	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	416/448 (92%)	0.39	8 (1%) 66 38	74, 102, 140, 166	0
1	B	416/448 (92%)	0.50	20 (4%) 30 11	73, 110, 157, 181	0
1	C	416/448 (92%)	0.42	11 (2%) 56 27	74, 103, 143, 174	0
1	D	416/448 (92%)	0.40	9 (2%) 62 33	73, 99, 135, 159	0
2	E	83/131 (63%)	0.45	6 (7%) 15 4	91, 119, 146, 160	0
2	F	79/131 (60%)	1.47	26 (32%) 0 0	132, 165, 184, 199	0
2	G	81/131 (61%)	0.89	13 (16%) 1 0	112, 139, 162, 171	0
2	H	80/131 (61%)	0.75	4 (5%) 28 10	102, 133, 159, 170	0
All	All	1987/2316 (85%)	0.50	97 (4%) 29 11	73, 108, 158, 199	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	132	GLN	6.2
2	G	66	TYR	4.6
1	C	420	TRP	4.4
1	B	403	LEU	4.4
1	B	402	LEU	4.1
2	F	99	GLU	4.0
2	F	79	LEU	4.0
1	B	342	HIS	3.8
1	D	420	TRP	3.7
1	C	342	HIS	3.7
2	G	137	ASN	3.5
2	G	106	HIS	3.5
2	F	72	PRO	3.5
2	F	70	SER	3.5
2	F	124	THR	3.4
2	G	80	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	141	TRP	3.3
1	B	420	TRP	3.2
2	H	74	ASP	3.2
2	F	128	MET	3.2
2	F	77	CYS	3.1
1	D	334	SER	3.1
2	E	66	TYR	3.1
1	C	402	LEU	3.1
1	D	342	HIS	3.1
2	F	100	SER	3.0
1	A	420	TRP	3.0
1	A	471	ASN	3.0
1	B	460	ALA	3.0
2	G	74	ASP	3.0
1	C	428	ILE	3.0
2	G	70	SER	2.9
2	F	123	GLY	2.9
2	E	124	THR	2.8
2	H	81	GLN	2.8
2	F	80	THR	2.8
2	H	128	MET	2.8
2	F	66	TYR	2.8
2	F	119	LYS	2.7
1	B	345	VAL	2.7
2	F	140	PRO	2.7
1	C	174	LYS	2.7
1	C	385	THR	2.7
2	E	61	VAL	2.6
1	A	82	TRP	2.6
1	C	82	TRP	2.6
2	F	71	LEU	2.5
2	G	85	HIS	2.5
1	B	373	SER	2.5
1	B	471	ASN	2.5
1	D	338	TYR	2.5
1	C	460	ALA	2.5
2	G	77	CYS	2.5
2	G	141	TRP	2.5
1	C	403	LEU	2.5
2	E	62	LEU	2.4
1	D	228	GLY	2.4
2	H	130	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	411	SER	2.4
2	G	140	PRO	2.3
1	B	139	ILE	2.3
2	F	97	ASN	2.3
1	C	139	ILE	2.3
2	F	130	CYS	2.3
2	F	93	ILE	2.3
1	B	452	HIS	2.3
2	E	95	HIS	2.3
2	F	114	CYS	2.3
2	E	137	ASN	2.2
1	C	228	GLY	2.2
1	B	218	GLY	2.2
1	D	82	TRP	2.2
1	B	390	SER	2.2
1	A	444	PHE	2.2
1	A	56	LEU	2.2
2	G	63	LEU	2.2
1	A	150	LEU	2.2
1	D	235	ASN	2.2
1	B	156	LEU	2.1
2	F	139	PRO	2.1
1	B	406	LYS	2.1
2	F	95	HIS	2.1
2	G	121	VAL	2.1
1	A	387	LYS	2.1
1	B	272	ILE	2.1
1	D	56	LEU	2.1
1	B	366	LEU	2.1
2	G	124	THR	2.1
2	F	110	CYS	2.1
1	B	181	GLY	2.1
2	F	117	ILE	2.1
2	F	109	TRP	2.0
2	F	81	GLN	2.0
1	D	294	LYS	2.0
1	B	63	SER	2.0
1	A	428	ILE	2.0
1	B	180	THR	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, 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
5	CA	D	506	1/1	0.35	0.25	143,143,143,143	0
3	NAG	C	502	14/15	0.56	0.23	124,132,139,141	0
3	NAG	D	501	14/15	0.64	0.21	127,132,134,136	0
3	NAG	A	502	14/15	0.66	0.23	113,137,146,147	0
3	NAG	A	501	14/15	0.67	0.20	146,156,158,158	0
3	NAG	B	502	14/15	0.68	0.27	130,139,153,156	0
3	NAG	D	502	14/15	0.69	0.28	101,124,136,138	0
3	NAG	C	501	14/15	0.70	0.20	161,167,171,172	0
4	EDO	B	504	4/4	0.76	0.38	76,76,79,79	0
5	CA	B	506	1/1	0.76	0.19	143,143,143,143	0
5	CA	A	506	1/1	0.76	0.27	125,125,125,125	0
3	NAG	B	501	14/15	0.80	0.17	175,177,178,181	0
4	EDO	D	504	4/4	0.81	0.54	63,71,73,74	0
4	EDO	C	504	4/4	0.81	0.73	76,80,81,84	0
4	EDO	A	504	4/4	0.85	0.90	80,81,83,83	0
5	CA	C	506	1/1	0.91	0.35	137,137,137,137	0
4	EDO	B	503	4/4	0.95	0.26	65,67,70,72	0
4	EDO	D	503	4/4	0.96	0.21	41,51,60,61	0
4	EDO	C	503	4/4	0.96	0.28	74,74,75,75	0
5	CA	D	505	1/1	0.97	0.16	70,70,70,70	0
5	CA	A	505	1/1	0.98	0.19	80,80,80,80	0
4	EDO	A	503	4/4	0.98	0.41	76,77,77,77	0
5	CA	C	505	1/1	0.98	0.12	63,63,63,63	0
5	CA	B	505	1/1	0.98	0.15	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.