



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:49 am BST

PDB ID : 6UTE
Title : Crystal structure of Z032 Fab in complex with WNV EDIII
Authors : Esswein, S.R.; Gristick, H.B.; Keeffe, J.R.; Bjorkman, P.J.
Deposited on : 2019-10-29
Resolution : 2.90 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 : 2.11
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) : 2.11

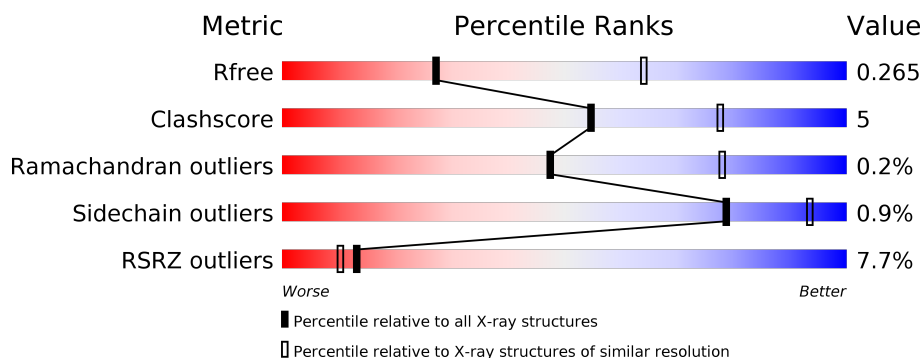
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	234	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	C	234	<div> <div>4%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	E	234	<div> <div>2%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	G	234	<div> <div>8%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	I	234	<div> <div>7%</div> <div>78%</div> <div>17%</div> <div>.</div> </div>
2	B	214	<div> <div>%</div> <div>85%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	214	<div><div></div><div>%</div><div>84%</div><div>15%</div></div>
2	F	214	<div><div></div><div>2%</div><div>85%</div><div>14%</div></div>
2	H	214	<div><div></div><div>22%</div><div>85%</div><div>13%</div><div></div></div>
2	J	214	<div><div></div><div>16%</div><div>85%</div><div>14%</div></div>
3	S	98	<div><div></div><div>26%</div><div>91%</div><div>9%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17255 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 Z032 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	219	Total	C	N	O	S	0	0	0
			1621	1023	270	322	6			
1	A	223	Total	C	N	O	S	0	0	0
			1651	1041	276	328	6			
1	E	220	Total	C	N	O	S	0	0	0
			1627	1026	271	324	6			
1	G	223	Total	C	N	O	S	0	0	0
			1651	1041	276	328	6			
1	I	224	Total	C	N	O	S	0	0	0
			1657	1044	277	330	6			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	221	HIS	-	expression tag	UNP S6B291
C	222	HIS	-	expression tag	UNP S6B291
C	223	HIS	-	expression tag	UNP S6B291
C	224	HIS	-	expression tag	UNP S6B291
C	225	HIS	-	expression tag	UNP S6B291
A	221	HIS	-	expression tag	UNP S6B291
A	222	HIS	-	expression tag	UNP S6B291
A	223	HIS	-	expression tag	UNP S6B291
A	224	HIS	-	expression tag	UNP S6B291
A	225	HIS	-	expression tag	UNP S6B291
E	221	HIS	-	expression tag	UNP S6B291
E	222	HIS	-	expression tag	UNP S6B291
E	223	HIS	-	expression tag	UNP S6B291
E	224	HIS	-	expression tag	UNP S6B291
E	225	HIS	-	expression tag	UNP S6B291
G	221	HIS	-	expression tag	UNP S6B291
G	222	HIS	-	expression tag	UNP S6B291
G	223	HIS	-	expression tag	UNP S6B291
G	224	HIS	-	expression tag	UNP S6B291

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Chain	Residue	Modelled	Actual	Comment	Reference
G	225	HIS	-	expression tag	UNP S6B291
I	221	HIS	-	expression tag	UNP S6B291
I	222	HIS	-	expression tag	UNP S6B291
I	223	HIS	-	expression tag	UNP S6B291
I	224	HIS	-	expression tag	UNP S6B291
I	225	HIS	-	expression tag	UNP S6B291

- Molecule 2 is a protein called Z032 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1662	1047	277	332	6			
2	B	213	Total	C	N	O	S	0	0	0
			1662	1047	277	332	6			
2	F	213	Total	C	N	O	S	0	0	0
			1662	1047	277	332	6			
2	H	210	Total	C	N	O	S	0	0	0
			1638	1029	274	329	6			
2	J	213	Total	C	N	O	S	0	0	0
			1662	1047	277	332	6			

- Molecule 3 is a protein called Envelope domain III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	98	Total	C	N	O	S	0	0	0
			732	467	125	138	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

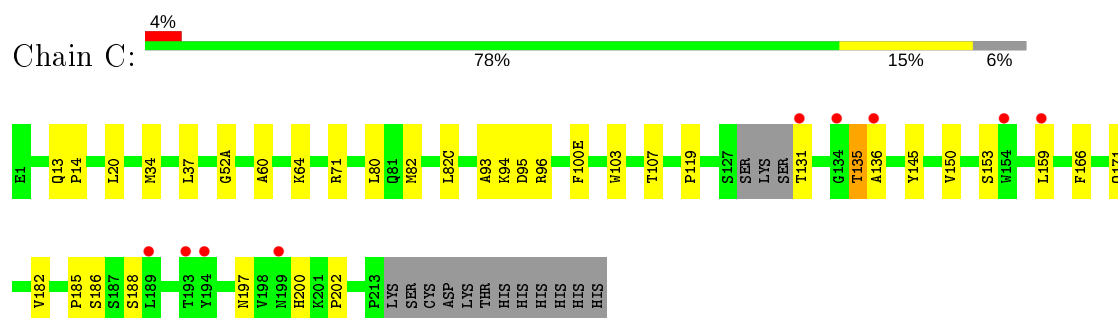


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

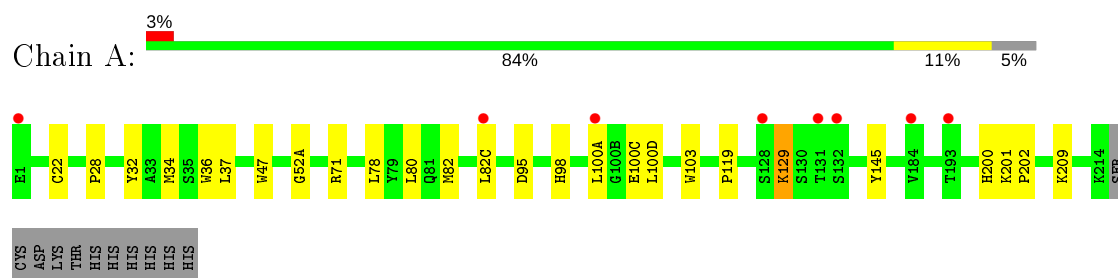
3 Residue-property plots [i](#)

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.

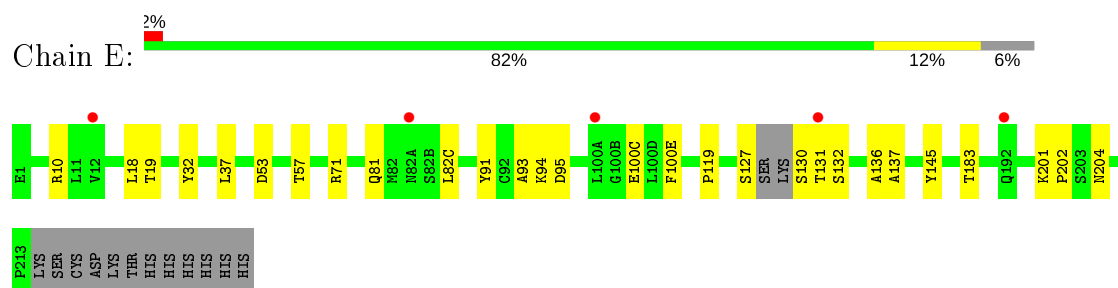
- Molecule 1: Z032 Fab heavy chain



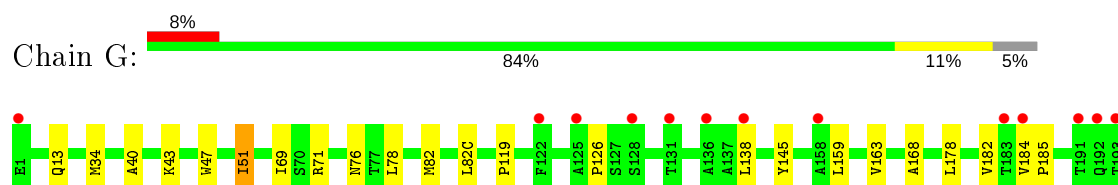
- Molecule 1: Z032 Fab heavy chain

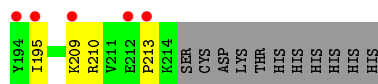


- Molecule 1: Z032 Fab heavy chain

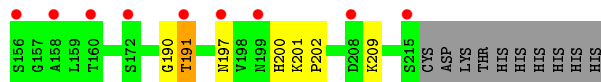
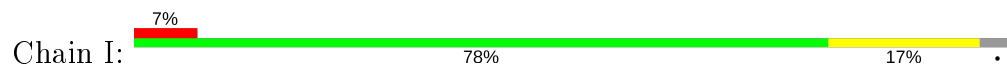


- Molecule 1: Z032 Fab heavy chain

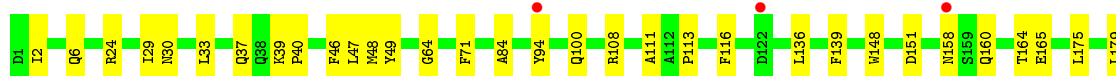
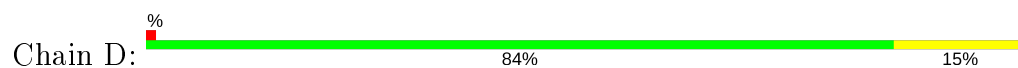




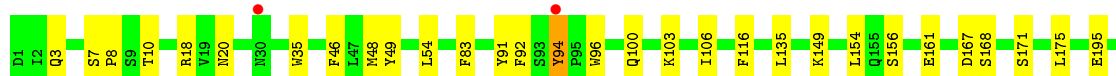
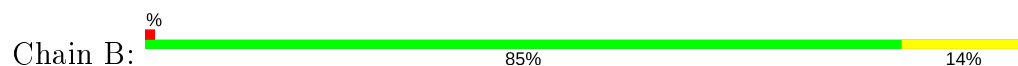
- Molecule 1: Z032 Fab heavy chain



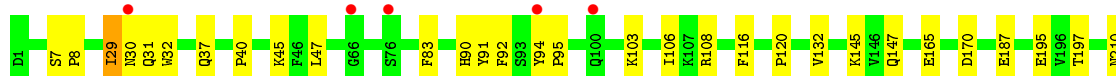
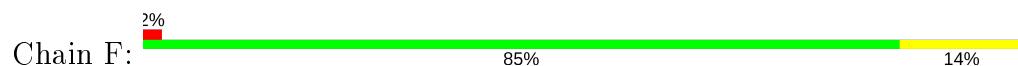
- Molecule 2: Z032 Fab light chain



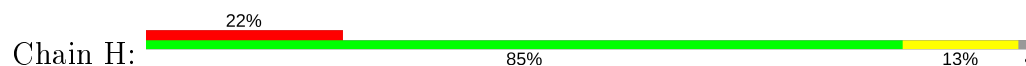
- Molecule 2: Z032 Fab light chain

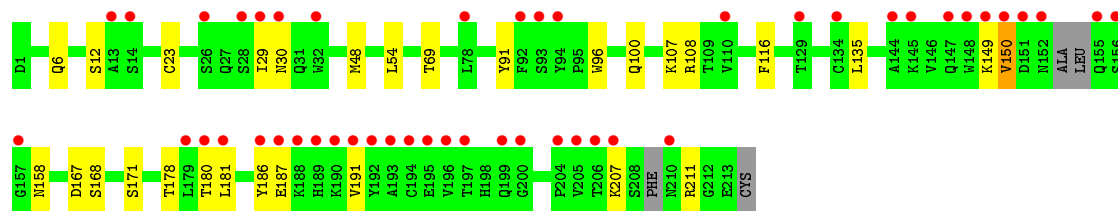


- Molecule 2: Z032 Fab light chain

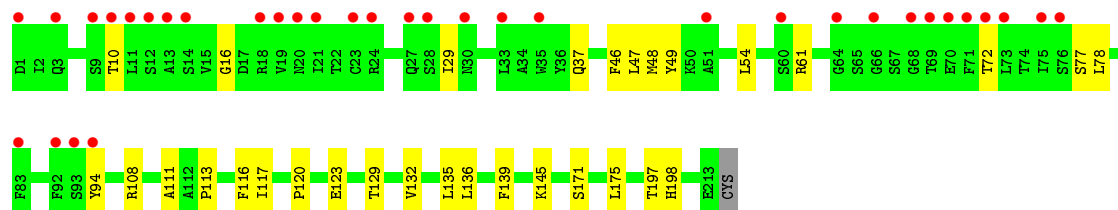
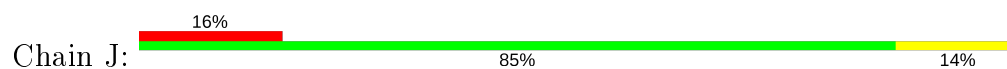


- Molecule 2: Z032 Fab light chain

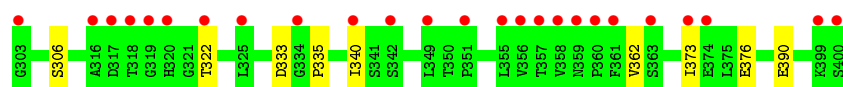
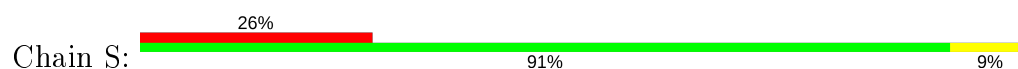




• Molecule 2: Z032 Fab light chain



• Molecule 3: Envelope domain III



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23 Å 114.02 Å 127.26 Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	39.99 – 2.90 39.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.99-2.90) 99.7 (39.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.90 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.223 , 0.264 0.223 , 0.265	Depositor DCC
R_{free} test set	2848 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: 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	0.25	0/1690	0.47	0/2302
1	C	0.25	0/1659	0.46	0/2261
1	E	0.25	0/1665	0.47	0/2269
1	G	0.25	0/1690	0.46	0/2302
1	I	0.24	0/1696	0.45	0/2310
2	B	0.25	0/1703	0.46	0/2313
2	D	0.25	0/1703	0.45	0/2313
2	F	0.25	0/1703	0.47	0/2313
2	H	0.24	0/1676	0.45	0/2273
2	J	0.25	0/1703	0.46	0/2313
3	S	0.24	0/750	0.45	0/1025
All	All	0.25	0/17638	0.46	0/23994

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	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	HIS	Peptide
2	F	30	ASN	Peptide

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	1651	0	1622	16	0
1	C	1621	0	1585	22	0
1	E	1627	0	1590	18	0
1	G	1651	0	1622	21	0
1	I	1657	0	1627	26	0
2	B	1662	0	1602	22	0
2	D	1662	0	1602	19	0
2	F	1662	0	1602	19	0
2	H	1638	0	1575	16	0
2	J	1662	0	1602	16	0
3	S	732	0	727	6	0
4	B	6	0	8	0	0
4	D	12	0	16	0	0
4	F	6	0	8	0	0
4	J	6	0	8	0	0
All	All	17255	0	16796	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 5.

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:E:131:THR:HG22	2:F:116:PHE:HB3	1.67	0.75
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.69	0.74
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.71	0.72
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.73	0.71
1:C:82:MET:HB3	1:C:82(C):LEU:HD21	1.75	0.69
2:J:16:GLY:H	2:J:78:LEU:HB3	1.58	0.69
1:C:171:GLN:HG2	2:D:160:GLN:HE22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:PRO:HB3	1:G:138:LEU:HB3	1.76	0.68
1:E:201:LYS:HG3	1:E:202:PRO:HD3	1.75	0.67
1:C:52(A):GLY:HA2	1:C:71:ARG:CZ	2.23	0.67
1:I:51:ILE:HG22	1:I:52(A):GLY:H	1.60	0.65
1:I:70:SER:HB2	1:I:79:TYR:HB2	1.79	0.64
2:F:40:PRO:HG2	2:F:165:GLU:HG2	1.79	0.64
1:A:82:MET:HB3	1:A:82(C):LEU:HD21	1.79	0.63
2:J:48:MET:HG2	2:J:54:LEU:HA	1.82	0.62
2:H:29:ILE:HG13	2:H:30:ASN:H	1.65	0.61
2:J:116:PHE:HB2	2:J:135:LEU:HB3	1.81	0.61
1:C:131:THR:HG22	2:D:116:PHE:HB3	1.83	0.60
2:D:2:ILE:HG21	2:D:29:ILE:HD11	1.83	0.60
1:G:82:MET:HB3	1:G:82(C):LEU:HD21	1.82	0.60
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.82	0.60
1:I:37:LEU:HD23	1:I:47:TRP:HA	1.84	0.60
1:C:93:ALA:HB1	1:C:100(E):PHE:HB3	1.82	0.59
1:I:32:TYR:O	1:I:71:ARG:NH1	2.35	0.59
2:H:187:GLU:HA	2:H:211:ARG:HH12	1.68	0.58
3:S:340:ILE:HD13	3:S:373:ILE:HG21	1.86	0.58
1:I:200:HIS:CD2	1:I:202:PRO:HD2	2.40	0.56
1:E:127:SER:O	1:E:130:SER:N	2.38	0.56
1:G:159:LEU:HD21	1:G:182:VAL:HG11	1.89	0.55
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.37	0.55
1:I:82:MET:HB3	1:I:82(C):LEU:HD21	1.88	0.54
1:G:168:ALA:HB2	1:G:178:LEU:HD23	1.88	0.54
2:H:116:PHE:HB2	2:H:135:LEU:HB3	1.88	0.54
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.88	0.54
1:E:131:THR:HA	2:F:116:PHE:HD1	1.73	0.54
1:G:195:ILE:HG22	1:G:210:ARG:HA	1.90	0.54
2:B:48:MET:HE3	2:B:54:LEU:HD12	1.90	0.53
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.90	0.53
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.90	0.53
2:D:40:PRO:HG2	2:D:165:GLU:HG2	1.91	0.53
2:F:29:ILE:HG12	2:F:90:HIS:HB2	1.89	0.53
2:D:46:PHE:HZ	2:D:49:TYR:HB3	1.74	0.53
1:C:153:SER:HB2	1:C:197:ASN:HB2	1.91	0.52
2:D:113:PRO:HB3	2:D:139:PHE:HB3	1.91	0.52
1:G:163:VAL:HG22	1:G:182:VAL:HG22	1.91	0.52
1:C:20:LEU:HD12	1:C:80:LEU:HD23	1.91	0.52
2:H:158:ASN:HD22	2:H:181:LEU:HD21	1.73	0.52
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:SER:HB2	1:G:76:ASN:HD21	1.75	0.52
2:B:100:GLN:NE2	1:E:57:THR:O	2.43	0.51
1:A:22:CYS:HB3	1:A:78:LEU:HB3	1.93	0.51
2:D:94:TYR:OH	3:S:306:SER:HB2	2.11	0.51
2:H:167:ASP:OD1	2:H:168:SER:N	2.43	0.51
1:G:185:PRO:HG3	1:I:191:THR:HA	1.93	0.51
1:A:100(A):LEU:HD22	2:B:94:TYR:HE2	1.76	0.50
1:E:19:THR:HG22	1:E:81:GLN:HG3	1.94	0.50
2:H:108:ARG:HD2	2:H:171:SER:HB2	1.94	0.50
2:J:145:LYS:HB3	2:J:197:THR:HB	1.92	0.50
2:F:29:ILE:HG13	2:F:92:PHE:HB2	1.94	0.50
2:B:116:PHE:HB2	2:B:135:LEU:HB3	1.92	0.49
2:J:46:PHE:HZ	2:J:49:TYR:HB3	1.76	0.49
2:B:3:GLN:HG2	2:F:95:PRO:HD3	1.94	0.49
1:C:94:LYS:HD2	1:C:95:ASP:O	2.12	0.49
1:G:34:MET:HB3	1:G:78:LEU:HD22	1.94	0.49
2:B:83:PHE:CG	2:B:106:ILE:HG12	2.47	0.49
1:E:94:LYS:HD2	1:E:95:ASP:O	2.12	0.49
1:G:209:LYS:NZ	1:G:210:ARG:O	2.45	0.49
1:A:52(A):GLY:HA2	1:A:71:ARG:CZ	2.43	0.49
1:I:34:MET:HB3	1:I:78:LEU:HD22	1.94	0.49
1:C:34:MET:HG2	1:C:71:ARG:NH1	2.28	0.49
1:I:51:ILE:HG21	1:I:71:ARG:HD2	1.95	0.49
2:B:35:TRP:HB2	2:B:48:MET:HG2	1.95	0.48
2:B:161:GLU:HB2	2:B:175:LEU:HD11	1.95	0.48
2:B:18:ARG:NH1	2:B:20:ASN:OD1	2.45	0.48
1:I:31:THR:O	1:I:99:SER:N	2.46	0.48
2:J:108:ARG:HH12	2:J:111:ALA:HB2	1.78	0.48
2:D:6:GLN:O	2:D:100:GLN:NE2	2.46	0.48
2:D:108:ARG:HH12	2:D:111:ALA:HB2	1.79	0.48
2:D:151:ASP:HA	2:D:191:VAL:HB	1.95	0.48
2:J:108:ARG:HD2	2:J:171:SER:HB2	1.96	0.48
1:E:93:ALA:HB1	1:E:100(E):PHE:HB3	1.95	0.47
1:I:47:TRP:NE1	1:I:49:SER:O	2.46	0.47
1:E:127:SER:N	1:E:131:THR:OG1	2.43	0.47
1:G:126:PRO:HG2	1:G:213:PRO:HA	1.95	0.47
1:A:201:LYS:HE3	1:I:10:ARG:HH12	1.77	0.47
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.96	0.47
1:C:135:THR:HG22	1:C:185:PRO:HA	1.96	0.47
2:J:136:LEU:HB2	2:J:175:LEU:HB3	1.96	0.47
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ALA:HB3	1:G:43:LYS:HD2	1.97	0.47
2:J:116:PHE:HD2	2:J:135:LEU:HD23	1.80	0.47
1:C:185:PRO:O	1:C:188:SER:OG	2.32	0.47
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.49	0.47
1:E:100(C):GLU:HB3	2:F:91:TYR:HB2	1.96	0.46
1:G:168:ALA:HA	1:G:178:LEU:HB3	1.97	0.46
1:C:136:ALA:HB2	1:C:186:SER:HA	1.98	0.46
1:C:96:ARG:NH1	3:S:390:GLU:OE1	2.48	0.46
1:A:28:PRO:HG2	1:A:32:TYR:HE1	1.81	0.46
2:F:103:LYS:NZ	2:F:165:GLU:OE2	2.42	0.46
2:D:48:MET:HE1	2:D:64:GLY:HA3	1.98	0.45
2:H:12:SER:HB3	2:H:107:LYS:HB2	1.98	0.45
1:A:209:LYS:HA	1:A:209:LYS:HD2	1.82	0.45
1:C:159:LEU:HD21	1:C:182:VAL:HG21	1.98	0.45
1:E:53:ASP:OD1	1:E:53:ASP:N	2.50	0.45
1:C:200:HIS:CD2	1:C:202:PRO:HD2	2.52	0.45
1:I:87:THR:HG23	1:I:110:THR:HA	1.98	0.45
1:A:100(C):GLU:HB2	2:B:91:TYR:HB2	1.98	0.45
2:F:210:ASN:HB2	2:F:213:GLU:HB3	1.99	0.45
1:G:182:VAL:HG12	1:G:184:VAL:HG23	1.99	0.45
1:I:36:TRP:CG	1:I:80:LEU:HD22	2.52	0.45
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.97	0.45
1:E:37:LEU:O	1:E:91:TYR:N	2.36	0.45
2:H:149:LYS:HD3	2:H:149:LYS:HA	1.60	0.44
2:H:186:TYR:O	2:H:211:ARG:NH1	2.50	0.44
2:H:91:TYR:HA	2:H:96:TRP:CE3	2.53	0.44
1:E:10:ARG:HH11	1:E:18:LEU:HD13	1.82	0.44
2:D:148:TRP:CG	2:D:179:LEU:HD13	2.53	0.44
3:S:322:THR:HG22	3:S:376:GLU:HB2	1.98	0.44
2:J:61:ARG:HD2	2:J:77:SER:O	2.18	0.43
2:F:145:LYS:HB3	2:F:197:THR:HB	2.00	0.43
2:H:207:LYS:HA	2:H:207:LYS:HD2	1.80	0.43
2:F:29:ILE:HG23	2:F:32:TRP:N	2.34	0.43
1:I:22:CYS:HB3	1:I:78:LEU:HB3	2.00	0.43
2:B:10:THR:HG22	2:B:103:LYS:HB3	2.00	0.43
1:A:47:TRP:CD1	2:B:96:TRP:HD1	2.37	0.43
2:B:167:ASP:OD1	2:B:168:SER:N	2.52	0.43
1:C:20:LEU:HD22	1:C:107:THR:HG21	2.01	0.43
2:D:39:LYS:HG2	2:D:84:ALA:HB2	1.99	0.43
2:F:37:GLN:O	2:F:45:LYS:N	2.48	0.43
1:G:34:MET:HG2	1:G:71:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:MET:HG2	2:H:54:LEU:HA	2.00	0.43
1:I:68:THR:HB	1:I:81:GLN:HB3	2.01	0.43
1:A:129:LYS:NZ	2:B:213:GLU:OE1	2.51	0.43
2:H:178:THR:HG22	2:H:180:THR:HG23	2.01	0.43
2:D:136:LEU:HB2	2:D:175:LEU:HB3	2.01	0.43
1:C:37:LEU:HD22	1:C:103:TRP:CH2	2.54	0.42
1:I:153:SER:O	1:I:197:ASN:N	2.43	0.42
1:E:32:TYR:O	1:E:71:ARG:NH1	2.50	0.42
2:D:24:ARG:HD3	2:B:92:PHE:CE2	2.55	0.42
1:I:130:SER:HB2	2:J:117:ILE:HG22	1.99	0.42
2:B:106:ILE:HD12	2:B:171:SER:HB3	2.02	0.42
1:C:60:ALA:O	1:C:64:LYS:HG3	2.20	0.42
1:C:94:LYS:HB3	1:C:94:LYS:HE3	1.76	0.42
2:B:156:SER:HB2	1:G:76:ASN:ND2	2.34	0.42
2:F:187:GLU:O	2:F:211:ARG:NH1	2.53	0.42
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.55	0.42
1:A:37:LEU:HD22	1:A:103:TRP:CH2	2.55	0.42
1:A:36:TRP:CE2	1:A:80:LEU:HB2	2.55	0.42
1:G:185:PRO:HG3	1:I:190:GLY:O	2.20	0.41
1:G:47:TRP:CD1	2:H:96:TRP:HD1	2.37	0.41
1:I:10:ARG:HG3	1:I:18:LEU:HD11	2.02	0.41
2:J:113:PRO:HD3	2:J:198:HIS:ND1	2.35	0.41
3:S:333:ASP:N	3:S:333:ASP:OD1	2.53	0.41
1:E:137:ALA:HB2	1:E:183:THR:HG22	2.03	0.41
3:S:335:PRO:HA	3:S:362:VAL:O	2.20	0.41
1:C:166:PHE:CD1	2:D:164:THR:HG23	2.55	0.41
2:B:46:PHE:HZ	2:B:49:TYR:HB3	1.86	0.41
1:C:13:GLN:HG3	1:C:14:PRO:HD2	2.02	0.41
2:F:83:PHE:CG	2:F:106:ILE:HG12	2.56	0.41
1:I:35:SER:HA	1:I:50:GLY:HA2	2.03	0.41
1:I:72:ASP:HB2	1:I:79:TYR:HE2	1.85	0.41
1:I:36:TRP:NE1	1:I:80:LEU:HB2	2.35	0.41
1:I:209:LYS:NZ	2:J:123:GLU:OE2	2.37	0.41
2:B:7:SER:HA	2:B:8:PRO:HA	1.84	0.41
1:E:132:SER:HA	1:E:136:ALA:HA	2.02	0.41
2:B:154:LEU:H	2:B:154:LEU:HD12	1.86	0.41
2:F:108:ARG:NH1	2:F:170:ASP:O	2.42	0.40
2:F:7:SER:HA	2:F:8:PRO:HA	1.92	0.40
1:A:95:ASP:HA	1:A:100(D):LEU:O	2.20	0.40
2:D:158:ASN:HD22	1:I:26:GLY:HA2	1.86	0.40
2:H:150:VAL:HG23	2:H:191:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:PRO:HB3	2:J:139:PHE:HB3	2.03	0.40
1:E:204:ASN:O	1:G:13:GLN:NE2	2.55	0.40
2:F:147:GLN:HB2	2:F:195:GLU:HB3	2.04	0.40
1:G:51:ILE:HG13	1:G:69:ILE:HG23	2.04	0.40
2:H:6:GLN:O	2:H:100:GLN:NE2	2.54	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	221/234 (94%)	208 (94%)	13 (6%)	0	100	100
1	C	215/234 (92%)	208 (97%)	7 (3%)	0	100	100
1	E	216/234 (92%)	211 (98%)	5 (2%)	0	100	100
1	G	221/234 (94%)	216 (98%)	5 (2%)	0	100	100
1	I	222/234 (95%)	214 (96%)	7 (3%)	1 (0%)	29	61
2	B	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
2	D	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	61
2	F	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	61
2	H	204/214 (95%)	195 (96%)	9 (4%)	0	100	100
2	J	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	29	61
3	S	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
All	All	2239/2338 (96%)	2146 (96%)	89 (4%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	30	ASN

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Mol	Chain	Res	Type
2	F	31	GLN
2	J	94	TYR
1	I	100	GLY

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	185/196 (94%)	184 (100%)	1 (0%)	88	96
1	C	181/196 (92%)	179 (99%)	2 (1%)	73	92
1	E	182/196 (93%)	181 (100%)	1 (0%)	88	96
1	G	185/196 (94%)	184 (100%)	1 (0%)	88	96
1	I	186/196 (95%)	183 (98%)	3 (2%)	62	86
2	B	188/189 (100%)	187 (100%)	1 (0%)	88	96
2	D	188/189 (100%)	188 (100%)	0	100	100
2	F	188/189 (100%)	186 (99%)	2 (1%)	73	92
2	H	186/189 (98%)	183 (98%)	3 (2%)	62	86
2	J	188/189 (100%)	184 (98%)	4 (2%)	53	81
3	S	82/82 (100%)	82 (100%)	0	100	100
All	All	1939/2007 (97%)	1921 (99%)	18 (1%)	78	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	135	THR
1	C	150	VAL
1	A	129	LYS
2	B	94	TYR
1	E	82(C)	LEU
2	F	29	ILE
2	F	94	TYR
1	G	51	ILE

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Mol	Chain	Res	Type
2	H	23	CYS
2	H	69	THR
2	H	150	VAL
1	I	1	GLU
1	I	191	THR
1	I	201	LYS
2	J	10	THR
2	J	29	ILE
2	J	72	THR
2	J	129	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	158	ASN
2	D	160	GLN
1	G	192	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	J	301	-	5,5,5	0.88	0	5,5,5	1.00	0
4	GOL	D	302	-	5,5,5	0.88	0	5,5,5	1.00	0
4	GOL	B	501	-	5,5,5	0.91	0	5,5,5	1.00	0
4	GOL	F	601	-	5,5,5	0.88	0	5,5,5	1.04	0
4	GOL	D	301	-	5,5,5	0.91	0	5,5,5	1.01	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	GOL	J	301	-	-	0/4/4/4	-
4	GOL	D	302	-	-	0/4/4/4	-
4	GOL	B	501	-	-	2/4/4/4	-
4	GOL	F	601	-	-	2/4/4/4	-
4	GOL	D	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	GOL	O1-C1-C2-C3
4	F	601	GOL	O1-C1-C2-O2
4	B	501	GOL	O1-C1-C2-C3
4	B	501	GOL	O1-C1-C2-O2

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	223/234 (95%)	0.39	8 (3%) 42 37	31, 48, 76, 84	0
1	C	219/234 (93%)	0.52	9 (4%) 37 32	35, 54, 82, 91	0
1	E	220/234 (94%)	0.34	5 (2%) 60 58	33, 44, 64, 74	0
1	G	223/234 (95%)	0.56	18 (8%) 12 9	34, 47, 113, 123	0
1	I	224/234 (95%)	0.72	17 (7%) 13 10	53, 71, 88, 102	0
2	B	213/214 (99%)	0.27	2 (0%) 84 84	30, 40, 62, 75	0
2	D	213/214 (99%)	0.43	3 (1%) 75 75	33, 46, 75, 83	0
2	F	213/214 (99%)	0.44	5 (2%) 60 58	37, 46, 57, 62	0
2	H	210/214 (98%)	1.31	47 (22%) 0 0	42, 69, 125, 139	0
2	J	213/214 (99%)	1.03	35 (16%) 1 1	46, 77, 98, 102	0
3	S	98/98 (100%)	1.28	25 (25%) 0 0	55, 77, 93, 105	0
All	All	2269/2338 (97%)	0.63	174 (7%) 13 10	30, 54, 95, 139	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	195	GLU	5.2
2	J	94	TYR	5.1
2	H	181	LEU	4.8
1	A	132	SER	4.8
2	J	19	VAL	4.6
2	F	76	SER	4.6
2	H	28	SER	4.6
2	H	192	TYR	4.5
2	H	152	ASN	4.4
2	H	156	SER	4.3
2	F	66	GLY	4.3
3	S	359	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	94	TYR	4.1
1	E	131	THR	4.0
2	D	158	ASN	4.0
2	H	194	CYS	4.0
1	C	131	THR	4.0
2	H	188	LYS	4.0
2	J	14	SER	4.0
1	I	191	THR	3.9
2	H	147	GLN	3.8
2	J	18	ARG	3.8
2	J	75	ILE	3.8
2	H	210	ASN	3.8
2	J	33	LEU	3.8
1	C	134	GLY	3.7
2	J	35	TRP	3.7
2	J	92	PHE	3.7
2	J	93	SER	3.6
2	H	157	GLY	3.6
2	H	187	GLU	3.6
2	J	11	LEU	3.6
2	H	186	TYR	3.6
2	H	155	GLN	3.5
3	S	357	THR	3.5
2	J	71	PHE	3.5
2	H	197	THR	3.5
2	J	23	CYS	3.4
3	S	355	LEU	3.4
2	H	149	LYS	3.4
2	J	20	ASN	3.4
1	G	128	SER	3.4
1	I	208	ASP	3.4
2	H	150	VAL	3.3
3	S	361	PHE	3.3
1	C	194	TYR	3.3
2	H	144	ALA	3.3
2	H	29	ILE	3.3
1	C	136	ALA	3.3
2	J	10	THR	3.2
1	C	154	TRP	3.2
1	I	99	SER	3.2
2	J	76	SER	3.2
2	H	179	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	196	VAL	3.2
3	S	317	ASP	3.2
2	J	13	ALA	3.1
2	J	28	SER	3.1
2	H	134	CYS	3.1
2	J	70	GLU	3.1
2	H	206	THR	3.0
1	I	100(A)	LEU	3.0
1	G	192	GLN	3.0
1	C	189	LEU	3.0
1	I	156	SER	3.0
1	A	1	GLU	3.0
2	H	148	TRP	2.9
1	G	193	THR	2.9
2	H	151	ASP	2.9
2	J	12	SER	2.9
2	F	30	ASN	2.9
2	H	14	SER	2.9
1	I	54	SER	2.9
2	J	51	ALA	2.9
2	H	145	LYS	2.9
2	H	191	VAL	2.9
2	D	122	ASP	2.8
2	D	94	TYR	2.8
3	S	325	LEU	2.8
1	A	128	SER	2.8
2	J	9	SER	2.8
3	S	322	THR	2.8
2	H	26	SER	2.8
3	S	374	GLU	2.7
2	J	73	LEU	2.7
2	J	30	ASN	2.7
3	S	316	ALA	2.7
1	G	213	PRO	2.7
3	S	318	THR	2.6
2	J	64	GLY	2.6
2	H	193	ALA	2.6
2	H	189	HIS	2.6
1	G	195	ILE	2.6
3	S	356	VAL	2.6
2	J	24	ARG	2.6
3	S	400	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	131	THR	2.6
1	I	1	GLU	2.6
3	S	342	SER	2.6
3	S	349	LEU	2.5
3	S	320	HIS	2.5
1	G	136	ALA	2.5
1	G	158	ALA	2.5
2	H	13	ALA	2.5
3	S	340	ILE	2.5
2	H	204	PRO	2.5
3	S	360	PRO	2.5
1	I	100	GLY	2.4
2	H	207	LYS	2.4
2	H	200	GLY	2.4
2	J	66	GLY	2.4
2	H	32	TRP	2.4
2	H	129	THR	2.4
2	J	83	PHE	2.4
2	B	94	TYR	2.4
2	J	69	THR	2.4
1	G	212	GLU	2.4
2	J	27	GLN	2.4
2	F	94	TYR	2.4
2	J	68	GLY	2.4
2	J	1	ASP	2.4
1	E	82(A)	ASN	2.4
3	S	399	LYS	2.4
1	G	1	GLU	2.3
1	G	209	LYS	2.3
1	C	159	LEU	2.3
1	G	191	THR	2.3
1	G	183	THR	2.3
3	S	303	GLY	2.3
2	H	199	GLN	2.3
1	G	184	VAL	2.2
1	A	100(A)	LEU	2.2
1	E	100(A)	LEU	2.2
1	E	192	GLN	2.2
3	S	334	GLY	2.2
2	J	21	ILE	2.2
1	I	79	TYR	2.2
1	G	122	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	190	LYS	2.2
3	S	358	VAL	2.2
2	J	3	GLN	2.2
2	H	93	SER	2.1
1	A	82(C)	LEU	2.1
2	B	30	ASN	2.1
2	H	30	ASN	2.1
2	H	110	VAL	2.1
3	S	319	GLY	2.1
2	H	92	PHE	2.1
1	I	158	ALA	2.1
3	S	351	PRO	2.1
1	I	215	SER	2.1
3	S	363	SER	2.1
1	C	193	THR	2.1
1	G	125	ALA	2.1
2	F	100	GLN	2.1
3	S	373	ILE	2.1
1	A	184	VAL	2.1
1	I	150	VAL	2.1
1	G	194	TYR	2.1
1	I	197	ASN	2.1
1	I	52	THR	2.1
1	I	172	SER	2.0
1	I	160	THR	2.0
2	H	180	THR	2.0
2	H	78	LEU	2.0
1	A	193	THR	2.0
2	J	72	THR	2.0
2	H	205	VAL	2.0
2	J	60	SER	2.0
1	E	12	VAL	2.0
1	G	131	THR	2.0
1	G	138	LEU	2.0
1	C	199	ASN	2.0
1	I	199	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	GOL	B	501	6/6	0.67	0.32	87,88,88,88	0
4	GOL	D	302	6/6	0.74	0.24	88,89,89,90	0
4	GOL	D	301	6/6	0.84	0.41	84,85,85,85	0
4	GOL	F	601	6/6	0.89	0.30	84,84,85,85	0
4	GOL	J	301	6/6	0.89	0.31	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.