Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2021 – 12:09 pm GMT

PDB ID	:	6ZER
Title	:	Crystal structure of receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with EY6A Fab
Authors	:	Zhou, D.; Zhao, Y.; Fry, E.E.; Ren, J.; Stuart, D.I.
Deposited on	:	2020-06-16
Resolution	:	3.80 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:

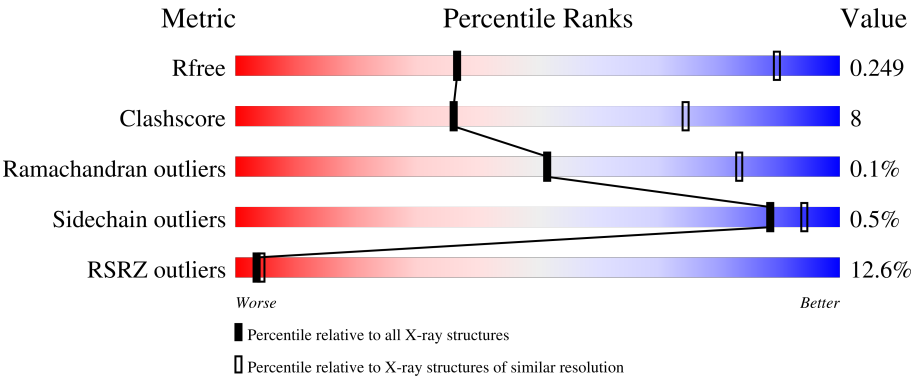
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	12% 74% 22% .
1	D	203	12% 75% 21% .
1	E	203	11% 76% 21% .
2	B	226	19% 77% 20% .
2	F	226	16% 78% 19% .

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Mol	Chain	Length	Quality of chain
2	H	226	12% 78% 20%
3	C	215	11% 87% 12%
3	G	215	9% 87% 13%
3	L	215	8% 87% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	601	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14647 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	197	Total	C	N	O	S	0	0	0
			1552	995	259	291	7			
1	A	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	D	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			

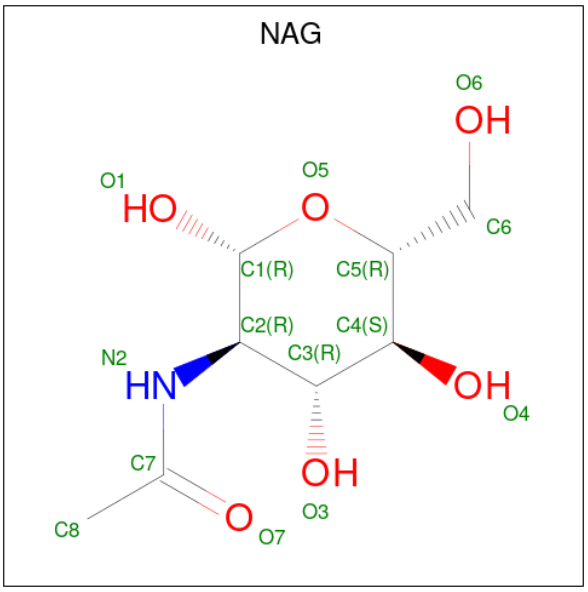
- Molecule 2 is a protein called EY6A heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1679	1065	281	326	7			
2	B	221	Total	C	N	O	S	0	0	0
			1679	1065	281	326	7			
2	F	220	Total	C	N	O	S	0	0	0
			1668	1058	279	324	7			

- Molecule 3 is a protein called EY6A light chain.

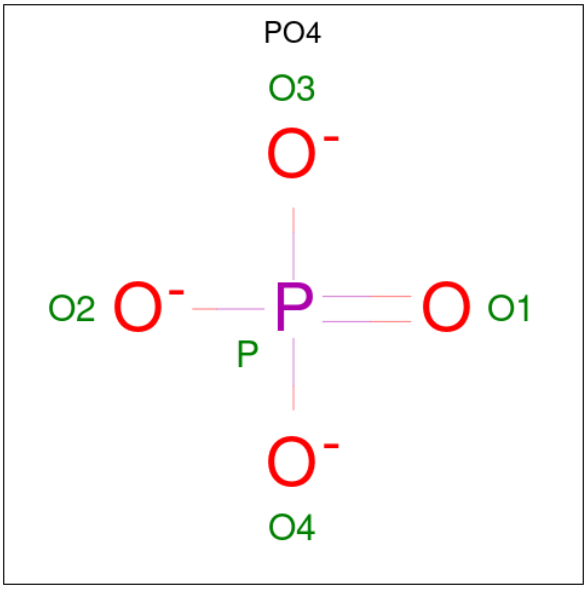
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1637	1022	273	336	6			
3	C	215	Total	C	N	O	S	0	0	0
			1637	1022	273	336	6			
3	G	215	Total	C	N	O	S	0	0	0
			1637	1022	273	336	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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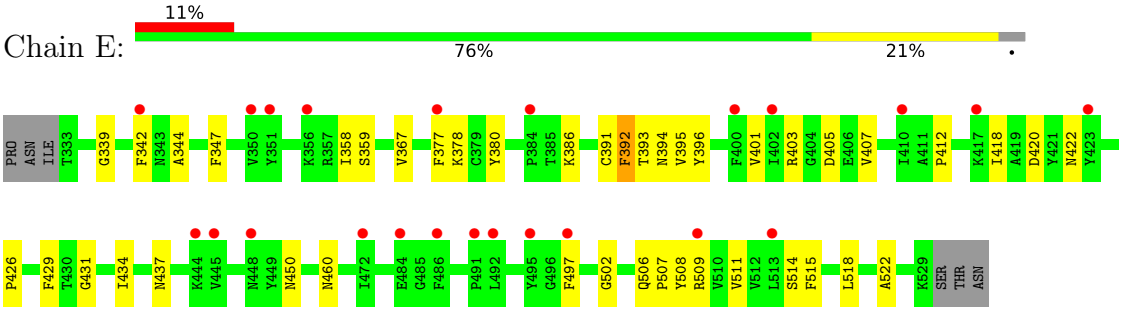
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	G	1	Total O P 5 4 1	0	0

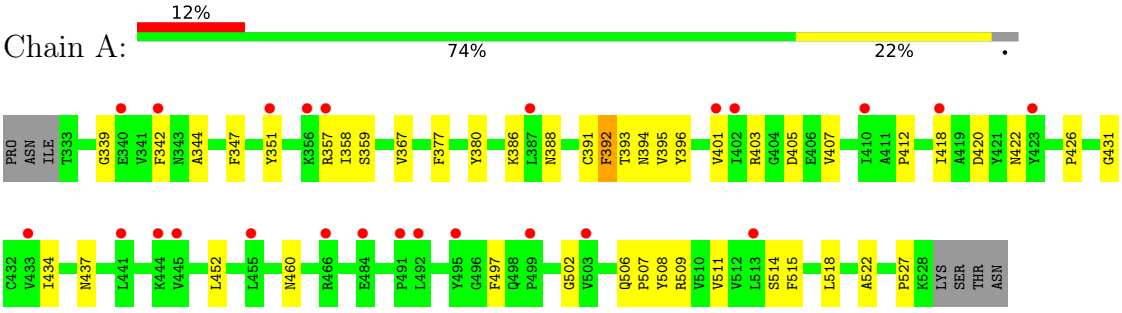
3 Residue-property plots (i)

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.

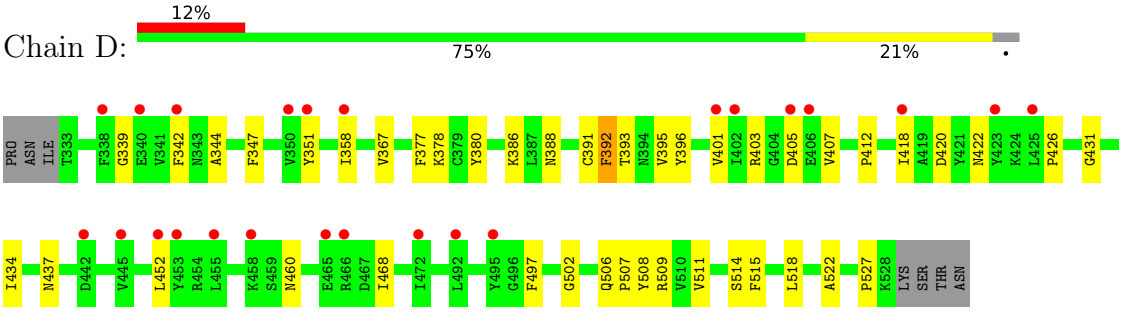
• Molecule 1: Spike protein S1



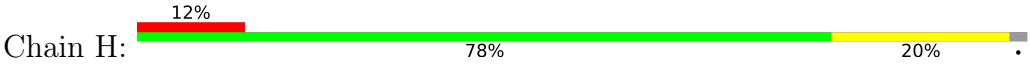
• Molecule 1: Spike protein S1

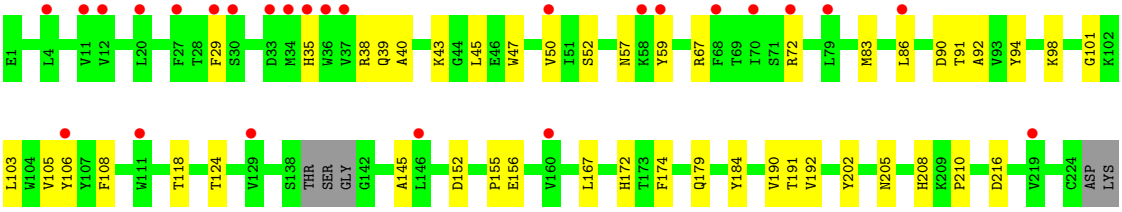


• Molecule 1: Spike protein S1

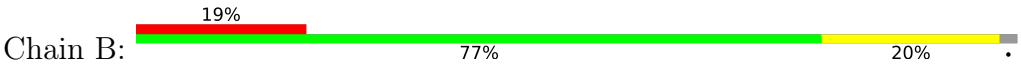


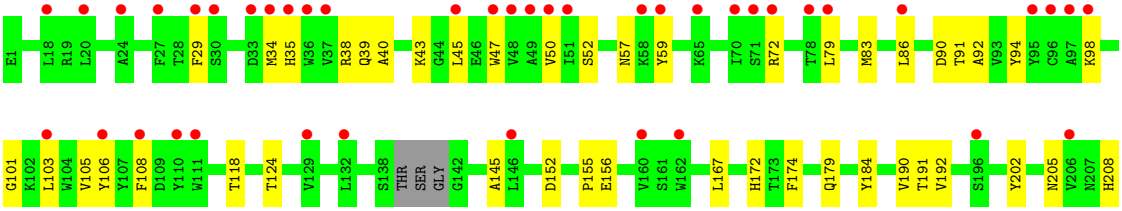
• Molecule 2: EY6A heavy chain



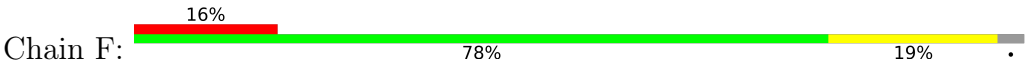


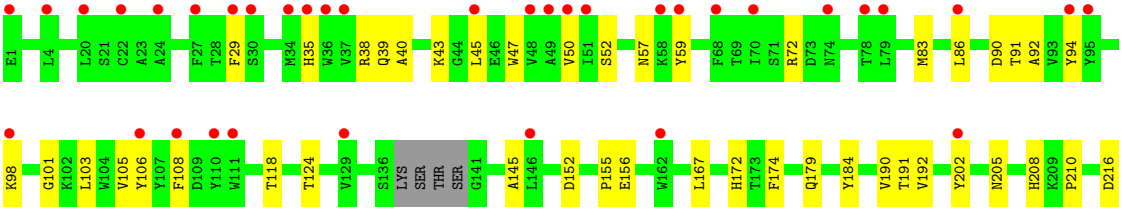
• Molecule 2: EY6A heavy chain



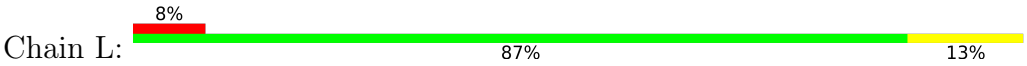


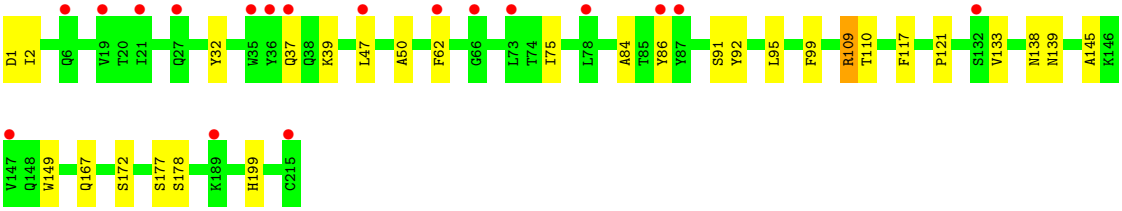
• Molecule 2: EY6A heavy chain



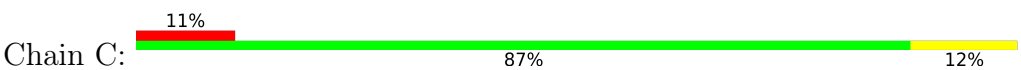


• Molecule 3: EY6A light chain

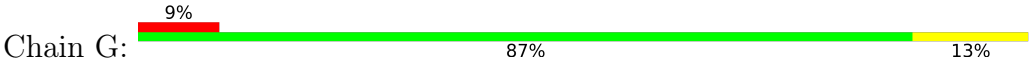


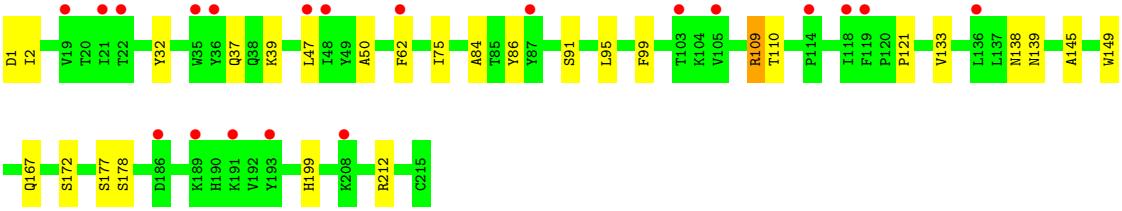


• Molecule 3: EY6A light chain



• Molecule 3: EY6A light chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.40Å 166.40Å 270.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.22 – 3.80 144.11 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.22-3.80) 99.9 (144.11-3.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.78Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.212 , 0.251 0.213 , 0.249	Depositor DCC
R_{free} test set	2176 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	159.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å^2)	185.0	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 32.99 % 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 8.5888e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PO4

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	0.28	0/1592	0.46	0/2168
1	D	0.29	0/1592	0.46	0/2168
1	E	0.29	0/1596	0.47	0/2174
2	B	0.27	0/1721	0.48	0/2342
2	F	0.27	0/1710	0.48	0/2328
2	H	0.28	0/1721	0.50	1/2342 (0.0%)
3	C	0.30	0/1670	0.47	0/2266
3	G	0.27	0/1670	0.47	0/2266
3	L	0.27	0/1670	0.47	0/2266
All	All	0.28	0/14942	0.47	1/20320 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	98	LYS	CD-CE-NZ	-5.09	99.99	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1548	0	1461	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1548	0	1461	34	0
1	E	1552	0	1462	34	0
2	B	1679	0	1636	34	0
2	F	1668	0	1621	32	0
2	H	1679	0	1636	33	0
3	C	1637	0	1595	20	0
3	G	1637	0	1595	20	0
3	L	1637	0	1595	21	0
4	A	14	0	13	2	0
4	D	14	0	13	2	0
4	E	14	0	13	2	0
5	C	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	1	0
5	L	5	0	0	0	0
All	All	14647	0	14101	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (230) 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)
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.70	0.73
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.70	0.72
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.70	0.72
3:G:212:ARG:NH2	5:G:301:PO4:O3	2.26	0.69
1:D:377:PHE:CD1	1:D:434:ILE:HG12	2.32	0.65
1:E:377:PHE:CD1	1:E:434:ILE:HG12	2.33	0.64
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.33	0.63
2:H:145:ALA:HB2	2:H:191:THR:HG22	1.82	0.62
2:H:172:HIS:HB3	2:H:174:PHE:HE1	1.64	0.62
2:B:145:ALA:HB2	2:B:191:THR:HG22	1.82	0.62
3:L:39:LYS:HD3	3:L:84:ALA:HB2	1.82	0.62
2:F:172:HIS:HB3	2:F:174:PHE:HE1	1.65	0.62
2:F:83:MET:HB3	2:F:86:LEU:HD21	1.81	0.61
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.81	0.61
2:B:172:HIS:HB3	2:B:174:PHE:HE1	1.64	0.61
2:F:92:ALA:HB3	2:F:94:TYR:HE1	1.66	0.61
1:E:358:ILE:HB	1:E:395:VAL:HB	1.83	0.61
2:H:92:ALA:HB3	2:H:94:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:LYS:HD3	3:C:84:ALA:HB2	1.83	0.60
2:B:92:ALA:HB3	2:B:94:TYR:HE1	1.66	0.60
3:G:39:LYS:HD3	3:G:84:ALA:HB2	1.83	0.60
1:E:342:PHE:HE1	1:E:511:VAL:HG11	1.66	0.60
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.83	0.60
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.81	0.60
1:E:392:PHE:HD2	1:E:515:PHE:HB3	1.66	0.60
1:A:358:ILE:HB	1:A:395:VAL:HB	1.83	0.60
1:A:392:PHE:HD2	1:A:515:PHE:HB3	1.66	0.60
2:F:145:ALA:HB2	2:F:191:THR:HG22	1.83	0.60
1:D:342:PHE:HE1	1:D:511:VAL:HG11	1.67	0.60
1:D:392:PHE:HD2	1:D:515:PHE:HB3	1.66	0.60
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.84	0.60
2:H:152:ASP:OD1	2:H:179:GLN:NE2	2.35	0.59
1:D:358:ILE:HB	1:D:395:VAL:HB	1.83	0.59
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.83	0.59
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.67	0.59
1:D:378:LYS:HA	3:G:95:LEU:HD12	1.85	0.59
1:E:392:PHE:CD2	1:E:515:PHE:HB3	2.38	0.59
1:A:392:PHE:CD2	1:A:515:PHE:HB3	2.38	0.59
1:D:392:PHE:CD2	1:D:515:PHE:HB3	2.38	0.59
2:B:152:ASP:OD1	2:B:179:GLN:NE2	2.36	0.58
1:D:377:PHE:HD1	1:D:434:ILE:HG12	1.68	0.58
2:F:152:ASP:OD1	2:F:179:GLN:NE2	2.36	0.58
1:D:377:PHE:HE2	2:F:59:TYR:HE1	1.52	0.57
2:F:156:GLU:HG2	2:F:184:TYR:CE2	2.39	0.57
1:E:377:PHE:HD1	1:E:434:ILE:HG12	1.69	0.57
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.69	0.57
1:D:386:LYS:HE3	2:F:101:GLY:HA2	1.85	0.57
2:B:156:GLU:HG2	2:B:184:TYR:CE2	2.39	0.57
2:F:52:SER:HB3	2:F:57:ASN:HB2	1.86	0.57
2:H:156:GLU:HG2	2:H:184:TYR:CE2	2.39	0.57
2:F:156:GLU:HG2	2:F:184:TYR:HE2	1.70	0.56
3:L:32:TYR:HB3	3:L:91:SER:HB2	1.87	0.56
2:H:52:SER:HB3	2:H:57:ASN:HB2	1.87	0.56
1:E:450:ASN:N	1:E:450:ASN:HD22	2.03	0.56
1:A:418:ILE:HD13	1:A:422:ASN:HD22	1.71	0.56
2:B:156:GLU:HG2	2:B:184:TYR:HE2	1.71	0.56
3:C:32:TYR:HB3	3:C:91:SER:HB2	1.87	0.56
1:E:418:ILE:HD13	1:E:422:ASN:HD22	1.71	0.56
2:B:52:SER:HB3	2:B:57:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:205:ASN:ND2	2:H:216:ASP:OD1	2.34	0.56
2:H:38:ARG:NH1	2:H:90:ASP:OD1	2.36	0.55
1:D:418:ILE:HD13	1:D:422:ASN:HD22	1.71	0.55
2:H:156:GLU:HG2	2:H:184:TYR:HE2	1.71	0.55
2:B:205:ASN:ND2	2:B:216:ASP:OD1	2.33	0.55
1:A:386:LYS:HE3	2:B:101:GLY:HA2	1.88	0.55
3:C:167:GLN:HE21	3:C:172:SER:HB3	1.72	0.55
3:G:32:TYR:HB3	3:G:91:SER:HB2	1.87	0.55
3:L:167:GLN:HE21	3:L:172:SER:HB3	1.72	0.55
1:A:391:CYS:C	1:A:392:PHE:HD1	2.10	0.55
1:D:391:CYS:C	1:D:392:PHE:HD1	2.10	0.54
2:F:205:ASN:ND2	2:F:216:ASP:OD1	2.34	0.54
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.89	0.54
1:E:391:CYS:C	1:E:392:PHE:HD1	2.11	0.54
2:B:108:PHE:HE2	3:C:99:PHE:HZ	1.53	0.54
3:G:167:GLN:HE21	3:G:172:SER:HB3	1.72	0.54
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.90	0.53
1:D:396:TYR:HB2	1:D:514:SER:OG	2.08	0.53
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.90	0.53
1:D:401:VAL:HG22	1:D:509:ARG:HG2	1.90	0.53
1:E:407:VAL:HG21	1:E:508:TYR:HD2	1.72	0.53
2:F:91:THR:HG23	2:F:118:THR:HA	1.91	0.53
1:A:407:VAL:HG21	1:A:508:TYR:HD2	1.73	0.53
2:B:91:THR:HG23	2:B:118:THR:HA	1.91	0.53
1:D:407:VAL:HG21	1:D:508:TYR:HD2	1.73	0.53
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.89	0.53
1:E:396:TYR:HB2	1:E:514:SER:OG	2.09	0.53
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.89	0.53
2:H:91:THR:HG23	2:H:118:THR:HA	1.91	0.53
1:A:396:TYR:HB2	1:A:514:SER:OG	2.09	0.53
2:B:167:LEU:HD21	2:B:190:VAL:HG21	1.91	0.52
2:H:167:LEU:HD21	2:H:190:VAL:HG21	1.91	0.52
2:F:167:LEU:HD21	2:F:190:VAL:HG21	1.91	0.52
2:H:208:HIS:CD2	2:H:210:PRO:HD2	2.45	0.52
2:B:208:HIS:CD2	2:B:210:PRO:HD2	2.45	0.52
2:F:208:HIS:CD2	2:F:210:PRO:HD2	2.45	0.52
1:E:377:PHE:HE2	2:H:59:TYR:HE1	1.57	0.51
1:A:377:PHE:HE2	2:B:59:TYR:HE1	1.59	0.51
1:E:344:ALA:HB3	1:E:347:PHE:HE1	1.76	0.51
2:F:191:THR:HG21	3:G:138:ASN:ND2	2.27	0.50
2:H:191:THR:HG21	3:L:138:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:VAL:HG21	4:E:601:NAG:H83	1.93	0.50
2:H:35:HIS:ND1	2:H:50:VAL:HG22	2.27	0.50
3:G:37:GLN:HG3	3:G:86:TYR:HE1	1.76	0.50
1:A:367:VAL:HG21	4:A:601:NAG:H83	1.93	0.50
2:B:35:HIS:ND1	2:B:50:VAL:HG22	2.27	0.50
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.77	0.50
1:D:367:VAL:HG21	4:D:601:NAG:H83	1.93	0.50
2:H:108:PHE:HE2	3:L:99:PHE:HZ	1.59	0.50
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.77	0.50
2:H:191:THR:HG21	3:L:138:ASN:HD22	1.76	0.50
3:L:37:GLN:HG3	3:L:86:TYR:HE1	1.76	0.50
3:C:37:GLN:HG3	3:C:86:TYR:HE1	1.76	0.50
1:D:393:THR:HA	1:D:522:ALA:HA	1.94	0.49
2:F:38:ARG:NH1	2:F:90:ASP:OD1	2.36	0.49
2:F:35:HIS:ND1	2:F:50:VAL:HG22	2.27	0.49
1:E:429:PHE:O	3:L:92:TYR:OH	2.20	0.49
3:G:1:ASP:OD1	3:G:2:ILE:N	2.44	0.49
2:F:45:LEU:HB2	3:G:99:PHE:CD2	2.47	0.49
2:B:38:ARG:NH1	2:B:90:ASP:OD1	2.36	0.48
3:G:145:ALA:HB2	3:G:199:HIS:HD2	1.78	0.48
1:D:437:ASN:HA	1:D:508:TYR:CD1	2.49	0.48
3:L:145:ALA:HB2	3:L:199:HIS:HD2	1.78	0.48
1:A:392:PHE:HD1	1:A:392:PHE:N	2.12	0.48
1:A:393:THR:HA	1:A:522:ALA:HA	1.94	0.48
3:G:121:PRO:HD3	3:G:133:VAL:HG22	1.96	0.48
1:E:437:ASN:HA	1:E:508:TYR:CD1	2.49	0.48
3:C:145:ALA:HB2	3:C:199:HIS:HD2	1.79	0.48
3:C:159:ASN:ND2	1:D:468:ILE:HD11	2.28	0.48
1:E:386:LYS:HE3	2:H:101:GLY:HA2	1.94	0.48
1:E:392:PHE:HD1	1:E:392:PHE:N	2.12	0.48
1:D:497:PHE:CE2	1:D:507:PRO:HB3	2.49	0.48
3:C:121:PRO:HD3	3:C:133:VAL:HG22	1.96	0.47
1:E:380:TYR:CE2	1:E:412:PRO:HD2	2.49	0.47
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.96	0.47
1:E:393:THR:HA	1:E:522:ALA:HA	1.95	0.47
1:A:437:ASN:HA	1:A:508:TYR:CD1	2.49	0.47
1:A:393:THR:HG21	1:A:518:LEU:H	1.79	0.47
1:D:392:PHE:HD1	1:D:392:PHE:N	2.12	0.47
3:G:62:PHE:CD1	3:G:75:ILE:HG12	2.50	0.47
1:E:393:THR:HG21	1:E:518:LEU:H	1.79	0.47
2:H:174:PHE:CE2	3:L:177:SER:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.49	0.47
1:D:392:PHE:N	1:D:392:PHE:CD1	2.83	0.47
3:G:149:TRP:NE1	3:G:178:SER:OG	2.35	0.47
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.49	0.47
2:H:103:LEU:HD11	3:L:50:ALA:HB2	1.96	0.47
2:B:191:THR:HG21	3:C:138:ASN:ND2	2.29	0.47
1:D:380:TYR:CE2	1:D:412:PRO:HD2	2.50	0.47
1:A:392:PHE:N	1:A:392:PHE:CD1	2.83	0.46
1:E:450:ASN:N	1:E:450:ASN:ND2	2.64	0.46
1:E:497:PHE:CE2	1:E:507:PRO:HB3	2.50	0.46
1:D:393:THR:HG21	1:D:518:LEU:H	1.80	0.46
2:H:29:PHE:O	2:H:72:ARG:NH2	2.48	0.46
2:B:29:PHE:O	2:B:72:ARG:NH2	2.48	0.46
3:L:1:ASP:OD1	3:L:2:ILE:N	2.45	0.46
3:C:62:PHE:CD1	3:C:75:ILE:HG12	2.50	0.46
3:C:149:TRP:NE1	3:C:178:SER:OG	2.35	0.46
1:E:392:PHE:N	1:E:392:PHE:CD1	2.83	0.46
3:C:1:ASP:OD1	3:C:2:ILE:N	2.45	0.46
2:F:191:THR:HG21	3:G:138:ASN:HD22	1.81	0.46
2:F:29:PHE:O	2:F:72:ARG:NH2	2.49	0.45
2:F:124:THR:HG22	2:F:155:PRO:HD3	1.98	0.45
2:H:124:THR:HG22	2:H:155:PRO:HD3	1.97	0.45
2:H:47:TRP:CZ2	2:H:50:VAL:HG23	2.52	0.45
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.51	0.45
2:B:47:TRP:CZ2	2:B:50:VAL:HG23	2.51	0.45
1:D:377:PHE:HE2	2:F:59:TYR:CE1	2.32	0.45
2:H:45:LEU:HB2	3:L:99:PHE:CD2	2.52	0.45
2:B:124:THR:HG22	2:B:155:PRO:HD3	1.98	0.44
2:F:108:PHE:HE2	3:G:99:PHE:HZ	1.66	0.44
2:F:47:TRP:CZ2	2:F:50:VAL:HG23	2.51	0.44
1:E:359:SER:OG	1:E:394:ASN:OD1	2.30	0.44
1:D:339:GLY:CA	4:D:601:NAG:H82	2.47	0.44
1:D:420:ASP:HB3	1:D:460:ASN:OD1	2.18	0.44
1:E:339:GLY:CA	4:E:601:NAG:H82	2.47	0.44
1:A:339:GLY:CA	4:A:601:NAG:H82	2.47	0.43
1:D:502:GLY:O	1:D:506:GLN:HG3	2.18	0.43
3:L:149:TRP:NE1	3:L:178:SER:OG	2.35	0.43
1:E:497:PHE:CD2	1:E:507:PRO:HB3	2.54	0.43
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.83	0.43
2:B:47:TRP:HZ2	2:B:50:VAL:HG23	1.84	0.43
2:B:191:THR:HG21	3:C:138:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:PHE:CD2	1:D:507:PRO:HB3	2.53	0.43
2:H:47:TRP:HZ2	2:H:50:VAL:HG23	1.84	0.43
1:A:359:SER:OG	1:A:394:ASN:OD1	2.31	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.18	0.43
2:F:47:TRP:HZ2	2:F:50:VAL:HG23	1.84	0.43
1:D:412:PRO:HB3	1:D:426:PRO:O	2.19	0.43
3:G:99:PHE:N	3:G:99:PHE:CD1	2.87	0.43
1:E:420:ASP:HB3	1:E:460:ASN:OD1	2.18	0.43
1:E:502:GLY:O	1:E:506:GLN:HG3	2.18	0.43
3:L:99:PHE:N	3:L:99:PHE:CD1	2.87	0.43
3:C:99:PHE:N	3:C:99:PHE:CD1	2.87	0.43
1:E:412:PRO:HB3	1:E:426:PRO:O	2.19	0.43
1:A:420:ASP:HB3	1:A:460:ASN:OD1	2.18	0.43
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.54	0.43
2:F:105:VAL:HG12	2:F:106:TYR:N	2.34	0.43
1:E:431:GLY:HA2	1:E:515:PHE:HD2	1.83	0.42
1:A:412:PRO:HB3	1:A:426:PRO:O	2.19	0.42
2:B:103:LEU:HD11	3:C:50:ALA:HB2	2.01	0.42
2:H:105:VAL:HG12	2:H:106:TYR:N	2.34	0.42
2:B:105:VAL:HG12	2:B:106:TYR:N	2.33	0.42
2:B:57:ASN:HB3	2:B:59:TYR:CE2	2.54	0.42
3:G:109:ARG:HD3	3:G:110:THR:O	2.20	0.42
1:D:431:GLY:HA2	1:D:515:PHE:HD2	1.84	0.42
2:F:192:VAL:HG11	2:F:202:TYR:CE1	2.54	0.42
2:H:57:ASN:HB3	2:H:59:TYR:CE2	2.55	0.42
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.33	0.42
2:H:192:VAL:HG11	2:H:202:TYR:CE1	2.54	0.42
2:F:57:ASN:HB3	2:F:59:TYR:CE2	2.55	0.42
2:H:145:ALA:HB3	3:L:117:PHE:CD2	2.55	0.42
2:B:192:VAL:HG11	2:B:202:TYR:CE1	2.54	0.42
2:B:45:LEU:HB2	3:C:99:PHE:CD2	2.55	0.41
1:D:403:ARG:NH1	1:D:405:ASP:HB2	2.35	0.41
1:A:403:ARG:NH1	1:A:405:ASP:HB2	2.34	0.41
3:L:109:ARG:HD3	3:L:110:THR:O	2.20	0.41
2:F:103:LEU:HD11	3:G:50:ALA:HB2	2.02	0.41
1:A:351:TYR:HE1	1:A:452:LEU:HB2	1.85	0.41
2:B:145:ALA:HB3	3:C:117:PHE:CD2	2.56	0.41
1:D:388:ASN:O	1:D:527:PRO:HD2	2.21	0.41
3:C:109:ARG:HD3	3:C:110:THR:O	2.20	0.41
2:B:174:PHE:CE2	3:C:177:SER:HB3	2.56	0.41
1:D:351:TYR:HE1	1:D:452:LEU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:403:ARG:NH1	1:E:405:ASP:HB2	2.35	0.41
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.86	0.41
1:A:388:ASN:O	1:A:527:PRO:HD2	2.21	0.41
1:A:377:PHE:HE2	2:B:59:TYR:CE1	2.37	0.41
2:F:174:PHE:CE2	3:G:177:SER:HB3	2.56	0.40
1:E:378:LYS:HA	3:L:95:LEU:HD12	2.03	0.40
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.04	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	194/203 (96%)	174 (90%)	20 (10%)	0	100	100
1	D	194/203 (96%)	174 (90%)	20 (10%)	0	100	100
1	E	195/203 (96%)	176 (90%)	19 (10%)	0	100	100
2	B	217/226 (96%)	205 (94%)	12 (6%)	0	100	100
2	F	216/226 (96%)	206 (95%)	10 (5%)	0	100	100
2	H	217/226 (96%)	206 (95%)	11 (5%)	0	100	100
3	C	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
3	G	213/215 (99%)	197 (92%)	15 (7%)	1 (0%)	29	66
3	L	213/215 (99%)	197 (92%)	15 (7%)	1 (0%)	29	66
All	All	1872/1932 (97%)	1732 (92%)	138 (7%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	139	ASN
3	G	139	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/176 (96%)	167 (99%)	1 (1%)	86	92
1	D	168/176 (96%)	167 (99%)	1 (1%)	86	92
1	E	167/176 (95%)	166 (99%)	1 (1%)	86	92
2	B	187/191 (98%)	186 (100%)	1 (0%)	88	94
2	F	185/191 (97%)	184 (100%)	1 (0%)	88	94
2	H	187/191 (98%)	187 (100%)	0	100	100
3	C	188/188 (100%)	187 (100%)	1 (0%)	88	94
3	G	188/188 (100%)	187 (100%)	1 (0%)	88	94
3	L	188/188 (100%)	187 (100%)	1 (0%)	88	94
All	All	1626/1665 (98%)	1618 (100%)	8 (0%)	88	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	392	PHE
3	L	109	ARG
1	A	392	PHE
2	B	98	LYS
3	C	109	ARG
1	D	392	PHE
2	F	98	LYS
3	G	109	ARG

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

Mol	Chain	Res	Type
1	E	450	ASN
1	A	450	ASN
3	C	161	GLN
1	D	450	ASN
3	G	161	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	NAG	D	601	1	14,14,15	0.37	0	17,19,21	0.41	0
5	PO4	L	301	-	4,4,4	0.91	0	6,6,6	0.44	0
5	PO4	F	301	-	4,4,4	0.90	0	6,6,6	0.44	0
5	PO4	G	301	-	4,4,4	0.95	0	6,6,6	0.40	0
4	NAG	E	601	1	14,14,15	0.35	0	17,19,21	0.45	0
4	NAG	A	601	1	14,14,15	0.36	0	17,19,21	0.45	0
5	PO4	C	301	-	4,4,4	0.92	0	6,6,6	0.43	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	NAG	D	601	1	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1

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	E	601	NAG	C1-C2-N2-C7
4	A	601	NAG	C1-C2-N2-C7
4	D	601	NAG	C1-C2-N2-C7
4	D	601	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	NAG	2	0
5	G	301	PO4	1	0
4	E	601	NAG	2	0
4	A	601	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/203 (96%)	0.78	24 (12%) 4 4	138, 202, 257, 312	0
1	D	196/203 (96%)	0.80	24 (12%) 4 4	133, 188, 235, 297	0
1	E	197/203 (97%)	0.77	23 (11%) 4 5	134, 192, 237, 295	0
2	B	221/226 (97%)	1.06	43 (19%) 1 1	126, 186, 234, 294	0
2	F	220/226 (97%)	1.03	37 (16%) 1 2	124, 183, 233, 280	0
2	H	221/226 (97%)	0.93	26 (11%) 4 5	127, 183, 234, 282	0
3	C	215/215 (100%)	0.81	24 (11%) 5 5	129, 174, 212, 268	0
3	G	215/215 (100%)	0.94	20 (9%) 8 7	121, 169, 209, 282	0
3	L	215/215 (100%)	0.84	18 (8%) 11 9	129, 169, 214, 312	0
All	All	1896/1932 (98%)	0.89	239 (12%) 3 4	121, 182, 234, 312	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	79	LEU	5.4
2	B	34	MET	5.2
2	F	78	THR	5.0
2	F	51	ILE	4.8
2	B	36	TRP	4.6
2	B	50	VAL	4.6
2	F	36	TRP	4.6
2	H	34	MET	4.6
2	H	106	TYR	4.6
3	G	36	TYR	4.6
2	H	27	PHE	4.5
2	B	79	LEU	4.5
2	F	58	LYS	4.4
2	B	51	ILE	4.3
2	H	79	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	30	SER	4.1
1	E	495	TYR	4.1
2	F	34	MET	4.0
1	A	401	VAL	4.0
2	B	70	ILE	4.0
2	B	27	PHE	3.9
2	F	50	VAL	3.9
1	A	402	ILE	3.8
1	A	423	TYR	3.8
2	F	68	PHE	3.7
2	B	45	LEU	3.7
2	F	27	PHE	3.7
2	B	35	HIS	3.6
2	B	58	LYS	3.5
3	C	36	TYR	3.5
3	L	62	PHE	3.5
1	A	444	LYS	3.5
3	L	36	TYR	3.5
2	B	97	ALA	3.4
1	A	445	VAL	3.4
2	B	29	PHE	3.4
1	D	342	PHE	3.4
1	A	342	PHE	3.3
2	B	96	CYS	3.3
1	A	466	ARG	3.3
1	D	423	TYR	3.3
2	H	146	LEU	3.3
1	E	351	TYR	3.2
2	B	108	PHE	3.2
2	H	36	TRP	3.2
1	E	497	PHE	3.2
2	F	1	GLU	3.2
1	E	484	GLU	3.2
2	B	48	VAL	3.2
2	F	37	VAL	3.1
2	B	206	VAL	3.1
2	B	210	PRO	3.1
2	B	78	THR	3.1
1	A	492	LEU	3.1
2	H	111	TRP	3.1
2	B	98	LYS	3.1
2	B	37	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	35	TRP	3.0
1	D	351	TYR	3.0
1	A	503	VAL	3.0
2	H	70	ILE	3.0
3	L	21	ILE	3.0
2	B	49	ALA	3.0
2	F	86	LEU	3.0
3	G	119	PHE	3.0
2	H	59	TYR	3.0
2	B	106	TYR	2.9
1	E	402	ILE	2.9
3	C	155	LEU	2.9
2	H	20	LEU	2.9
3	L	47	LEU	2.9
1	D	401	VAL	2.9
2	H	58	LYS	2.9
1	E	410	ILE	2.9
1	A	495	TYR	2.9
3	G	87	TYR	2.8
2	F	108	PHE	2.8
2	H	50	VAL	2.8
1	A	340	GLU	2.8
3	L	215	CYS	2.8
3	C	21	ILE	2.8
3	C	103	THR	2.8
1	E	509	ARG	2.8
3	G	21	ILE	2.7
2	B	111	TRP	2.7
3	G	19	VAL	2.7
1	E	423	TYR	2.7
1	E	445	VAL	2.7
3	C	159	ASN	2.7
1	E	350	VAL	2.7
1	A	410	ILE	2.7
3	C	37	GLN	2.7
3	C	62	PHE	2.7
2	H	219	VAL	2.7
1	D	340	GLU	2.6
1	D	453	TYR	2.6
3	C	47	LEU	2.6
1	A	356	LYS	2.6
1	E	472	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	30	SER	2.6
2	B	20	LEU	2.6
2	F	24	ALA	2.6
2	H	72	ARG	2.6
1	A	433	VAL	2.6
3	L	189	LYS	2.6
3	L	86	TYR	2.6
3	G	47	LEU	2.6
2	H	68	PHE	2.6
3	G	35	TRP	2.5
3	C	87	TYR	2.5
1	E	448	ASN	2.5
1	A	441	LEU	2.5
1	E	356	LYS	2.5
2	F	59	TYR	2.5
2	F	22	CYS	2.5
2	F	129	VAL	2.5
2	H	37	VAL	2.5
1	A	484	GLU	2.5
3	L	37	GLN	2.5
1	D	402	ILE	2.5
1	D	465	GLU	2.4
2	B	103	LEU	2.4
1	D	350	VAL	2.4
1	D	455	LEU	2.4
2	F	74	ASN	2.4
2	H	35	HIS	2.4
2	F	219	VAL	2.4
3	L	132	SER	2.4
3	G	208	LYS	2.4
2	B	65	LYS	2.4
1	E	492	LEU	2.4
3	C	116	VAL	2.4
1	E	377	PHE	2.4
2	F	30	SER	2.4
3	C	143	ARG	2.4
2	F	45	LEU	2.4
1	D	338	PHE	2.4
3	C	86	TYR	2.4
1	E	513	LEU	2.4
2	B	86	LEU	2.4
3	C	19	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	458	LYS	2.4
1	D	466	ARG	2.3
2	H	86	LEU	2.3
1	E	444	LYS	2.3
1	D	418	ILE	2.3
1	A	455	LEU	2.3
3	G	114	PRO	2.3
1	A	351	TYR	2.3
2	F	162	TRP	2.3
1	D	472	ILE	2.3
2	B	59	TYR	2.3
2	B	160	VAL	2.3
2	F	94	TYR	2.3
2	F	110	TYR	2.3
3	L	147	VAL	2.3
3	L	78	LEU	2.3
3	C	46	LEU	2.3
1	A	499	PRO	2.3
3	C	211	ASN	2.3
2	H	29	PHE	2.3
2	F	29	PHE	2.3
2	F	20	LEU	2.3
2	F	95	TYR	2.3
3	C	32	TYR	2.3
1	E	486	PHE	2.3
2	B	72	ARG	2.3
2	B	196	SER	2.3
3	G	62	PHE	2.3
1	E	400	PHE	2.3
1	E	384	PRO	2.2
2	H	4	LEU	2.2
3	G	186	ASP	2.2
1	D	425	LEU	2.2
1	D	452	LEU	2.2
2	F	146	LEU	2.2
2	B	146	LEU	2.2
1	A	357	ARG	2.2
1	A	387	LEU	2.2
1	D	495	TYR	2.2
3	L	87	TYR	2.2
1	D	492	LEU	2.2
1	D	405	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	24	ALA	2.2
3	G	118	ILE	2.2
2	H	12	VAL	2.2
3	L	19	VAL	2.2
2	H	33	ASP	2.2
2	B	33	ASP	2.2
3	G	22	THR	2.2
3	C	24	ARG	2.2
1	D	442	ASP	2.2
3	G	189	LYS	2.2
1	E	491	PRO	2.2
1	A	418	ILE	2.2
2	F	106	TYR	2.2
1	E	417	LYS	2.2
3	L	66	GLY	2.2
2	B	162	TRP	2.2
2	F	111	TRP	2.2
3	C	48	ILE	2.2
1	D	358	ILE	2.2
2	B	110	TYR	2.1
2	H	11	VAL	2.1
2	F	48	VAL	2.1
2	B	71	SER	2.1
2	F	70	ILE	2.1
3	L	27	GLN	2.1
1	D	445	VAL	2.1
2	F	35	HIS	2.1
2	F	98	LYS	2.1
2	H	129	VAL	2.1
2	B	95	TYR	2.1
3	G	136	LEU	2.1
2	B	132	LEU	2.1
2	F	4	LEU	2.1
3	C	162	GLU	2.1
2	F	49	ALA	2.1
3	L	35	TRP	2.1
3	C	114	PRO	2.1
2	B	47	TRP	2.1
2	F	202	TYR	2.1
1	D	406	GLU	2.1
2	B	18	LEU	2.1
3	C	197	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	48	ILE	2.0
3	L	6	GLN	2.0
3	C	119	PHE	2.0
3	G	103	THR	2.0
1	A	491	PRO	2.0
1	A	513	LEU	2.0
2	B	129	VAL	2.0
2	H	160	VAL	2.0
3	G	191	LYS	2.0
3	C	95	LEU	2.0
3	G	105	VAL	2.0
3	G	193	TYR	2.0
3	L	73	LEU	2.0
1	E	342	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	601	14/15	0.63	0.53	176,266,291,298	0
4	NAG	D	601	14/15	0.63	0.36	157,263,287,296	0
5	PO4	C	301	5/5	0.65	0.23	193,202,239,260	0
4	NAG	E	601	14/15	0.67	0.26	181,258,279,296	0
5	PO4	G	301	5/5	0.82	0.28	172,193,212,246	0
5	PO4	F	301	5/5	0.86	0.23	200,205,271,272	0
5	PO4	L	301	5/5	0.86	0.21	167,198,240,250	0

6.5 Other polymers (i)

There are no such residues in this entry.