



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 AM UTC

PDB ID : 7A5A / pdb_00007a5a
Title : Crimean-Congo Hemorrhagic Fever Virus Envelope Glycoprotein Gc W1191H/W1197A/W1199A Mutant in Postfusion Conformation (Monoclinic Crystal Form)
Authors : Hellert, J.; Guardado-Calvo, P.; Rey, F.A.
Deposited on : 2020-08-20
Resolution : 2.99 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

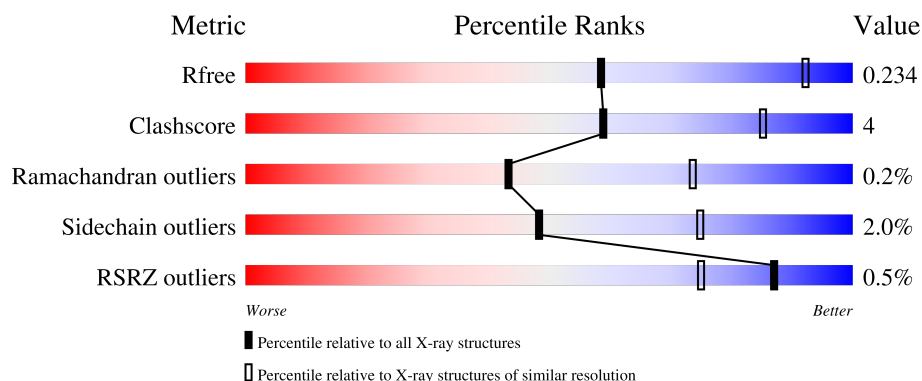
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 $\leq 5\%$. 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	540	 82% 11% 6%
1	B	540	 81% 13% 6%
1	C	540	 82% 10% 8%
1	D	540	 80% 13% 8%
1	E	540	 78% 14% 8%

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Mol	Chain	Length	Quality of chain
1	F	540	79% 13% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23452 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3918	2454	669	760	35			
1	B	505	Total	C	N	O	S	0	0	0
			3918	2454	669	760	35			
1	C	498	Total	C	N	O	S	0	0	0
			3866	2423	660	748	35			
1	D	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			
1	E	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			
1	F	499	Total	C	N	O	S	0	0	0
			3873	2427	661	750	35			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	TRP	-	expression tag	UNP Q8JSZ3
A	1034	SER	-	expression tag	UNP Q8JSZ3
A	1035	HIS	-	expression tag	UNP Q8JSZ3
A	1036	PRO	-	expression tag	UNP Q8JSZ3
A	1037	GLN	-	expression tag	UNP Q8JSZ3
A	1038	PHE	-	expression tag	UNP Q8JSZ3
A	1039	GLU	-	expression tag	UNP Q8JSZ3
A	1040	LYS	-	expression tag	UNP Q8JSZ3
A	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
A	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1033	TRP	-	expression tag	UNP Q8JSZ3
B	1034	SER	-	expression tag	UNP Q8JSZ3
B	1035	HIS	-	expression tag	UNP Q8JSZ3
B	1036	PRO	-	expression tag	UNP Q8JSZ3
B	1037	GLN	-	expression tag	UNP Q8JSZ3
B	1038	PHE	-	expression tag	UNP Q8JSZ3

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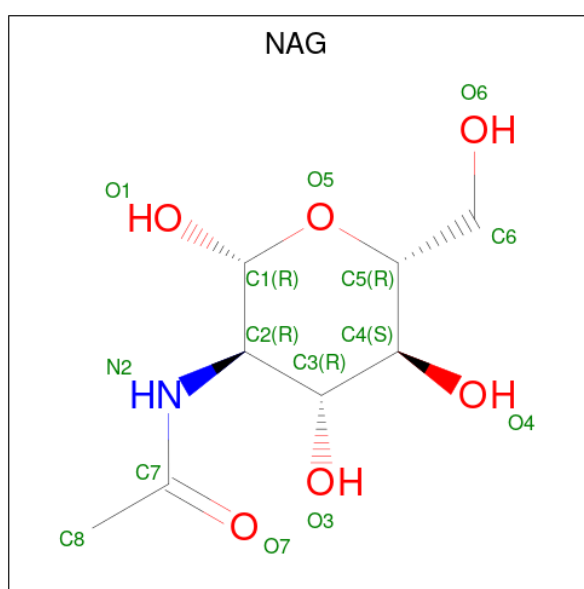
Chain	Residue	Modelled	Actual	Comment	Reference
B	1039	GLU	-	expression tag	UNP Q8JSZ3
B	1040	LYS	-	expression tag	UNP Q8JSZ3
B	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
B	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1033	TRP	-	expression tag	UNP Q8JSZ3
C	1034	SER	-	expression tag	UNP Q8JSZ3
C	1035	HIS	-	expression tag	UNP Q8JSZ3
C	1036	PRO	-	expression tag	UNP Q8JSZ3
C	1037	GLN	-	expression tag	UNP Q8JSZ3
C	1038	PHE	-	expression tag	UNP Q8JSZ3
C	1039	GLU	-	expression tag	UNP Q8JSZ3
C	1040	LYS	-	expression tag	UNP Q8JSZ3
C	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
C	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
D	1033	TRP	-	expression tag	UNP Q8JSZ3
D	1034	SER	-	expression tag	UNP Q8JSZ3
D	1035	HIS	-	expression tag	UNP Q8JSZ3
D	1036	PRO	-	expression tag	UNP Q8JSZ3
D	1037	GLN	-	expression tag	UNP Q8JSZ3
D	1038	PHE	-	expression tag	UNP Q8JSZ3
D	1039	GLU	-	expression tag	UNP Q8JSZ3
D	1040	LYS	-	expression tag	UNP Q8JSZ3
D	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
D	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
D	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
E	1033	TRP	-	expression tag	UNP Q8JSZ3
E	1034	SER	-	expression tag	UNP Q8JSZ3
E	1035	HIS	-	expression tag	UNP Q8JSZ3
E	1036	PRO	-	expression tag	UNP Q8JSZ3
E	1037	GLN	-	expression tag	UNP Q8JSZ3
E	1038	PHE	-	expression tag	UNP Q8JSZ3
E	1039	GLU	-	expression tag	UNP Q8JSZ3
E	1040	LYS	-	expression tag	UNP Q8JSZ3
E	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
E	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
E	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
F	1033	TRP	-	expression tag	UNP Q8JSZ3
F	1034	SER	-	expression tag	UNP Q8JSZ3
F	1035	HIS	-	expression tag	UNP Q8JSZ3
F	1036	PRO	-	expression tag	UNP Q8JSZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1037	GLN	-	expression tag	UNP Q8JSZ3
F	1038	PHE	-	expression tag	UNP Q8JSZ3
F	1039	GLU	-	expression tag	UNP Q8JSZ3
F	1040	LYS	-	expression tag	UNP Q8JSZ3
F	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
F	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
F	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

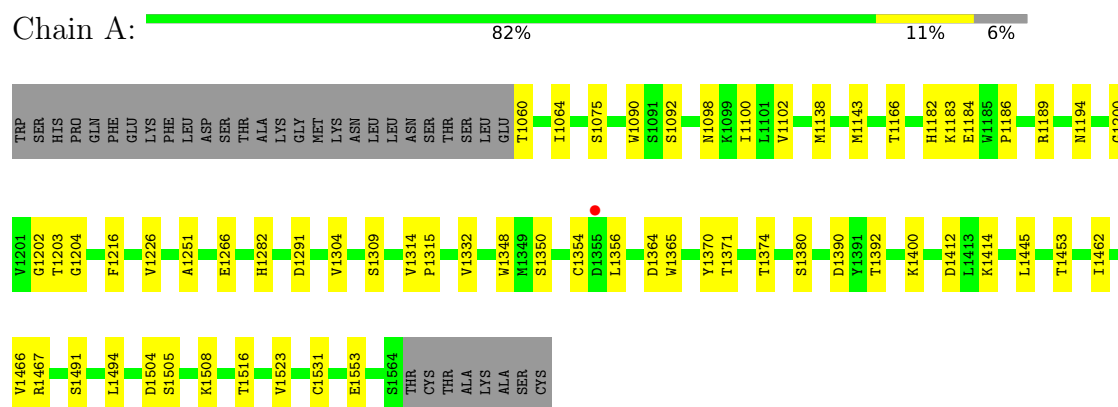
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	D	2	Total	Cl	0	0
			2	2		

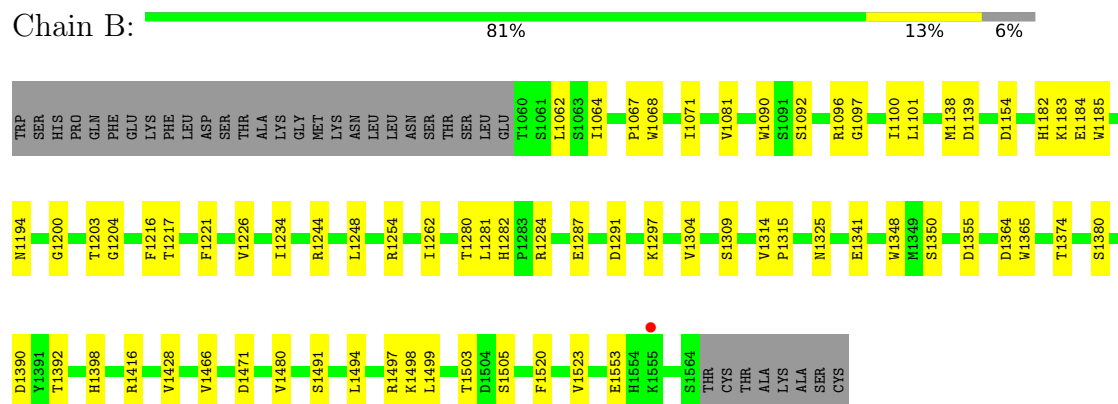
3 Residue-property plots

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.

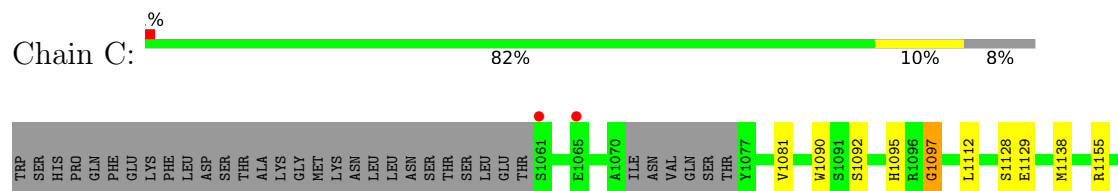
• Molecule 1: Envelopment polypeptide

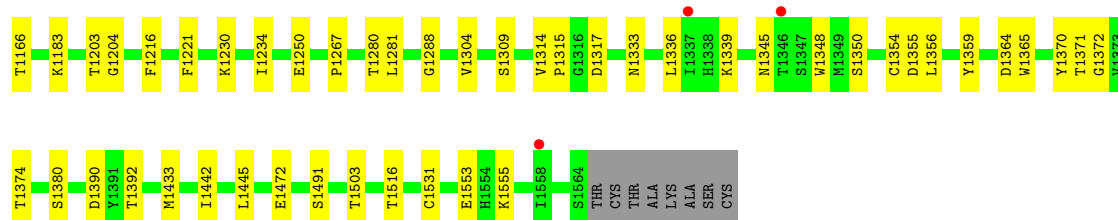


• Molecule 1: Envelopment polypeptide

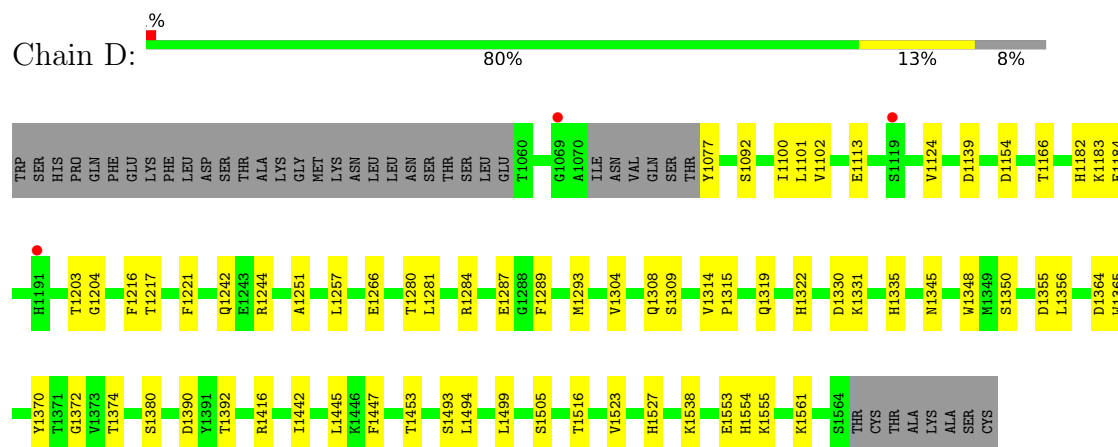


• Molecule 1: Envelopment polypeptide

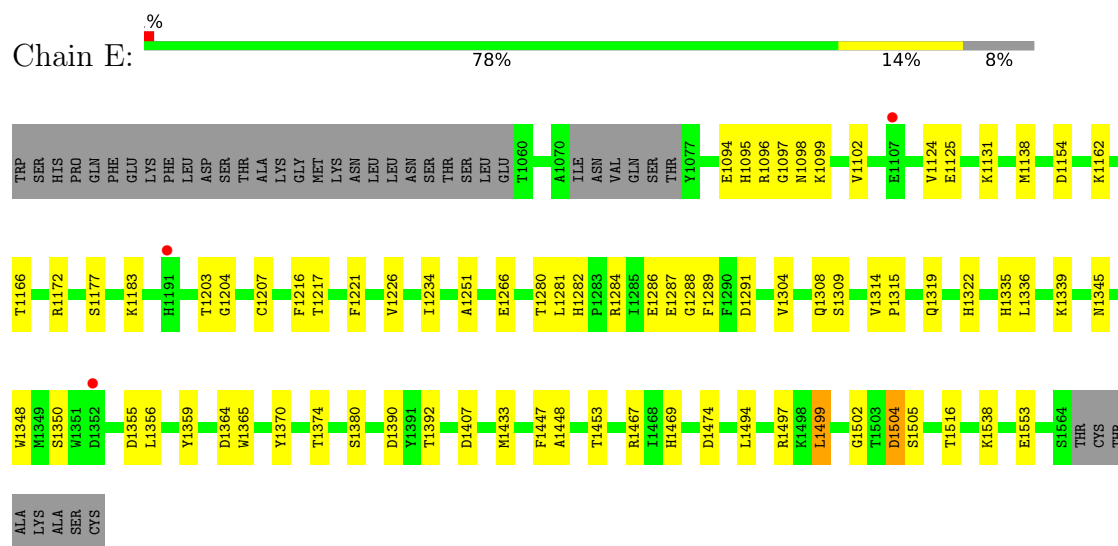




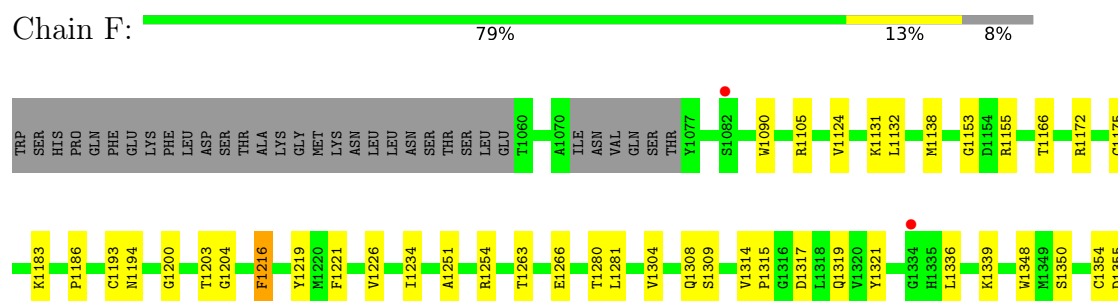
• Molecule 1: Envelopment polyprotein



• Molecule 1: Envelopment polyprotein



• Molecule 1: Envelopment polyprotein



L1356	D1364	Y1370	T1374	S1380	L1385	D1390	Y1391	T1392	K1393	F1397	K1400	D1412	E1429	M1433	E1434	K1438	K1465	D1474	S1491	L1494	D1504	S1505	T1516	S1549	E1553	S1564	THR	CYS	THR	ALA	LYS	ALA	SER	CYS
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.97Å 108.26Å 223.53Å 90.00° 93.22° 90.00°	Depositor
Resolution (Å)	49.05 – 2.99 49.05 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.05-2.99) 91.0 (49.05-2.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.204 , 0.239 0.203 , 0.234	Depositor DCC
R_{free} test set	2001 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23452	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/4005	0.36	0/5432
1	B	0.21	0/4005	0.37	0/5432
1	C	0.19	0/3952	0.36	0/5357
1	D	0.13	0/3959	0.34	0/5367
1	E	0.13	0/3959	0.34	0/5367
1	F	0.14	0/3959	0.35	0/5367
All	All	0.17	0/23839	0.36	0/32322

There are no bond length outliers.

There are no bond angle outliers.

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	3918	0	3810	32	0
1	B	3918	0	3810	38	0
1	C	3866	0	3756	31	0
1	D	3873	0	3764	40	0
1	E	3873	0	3764	42	0
1	F	3873	0	3764	40	0
2	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	26	1	0
2	C	28	0	26	0	0
2	D	14	0	13	1	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	23452	0	22785	204	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 4.

All (204) 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:1355:ASP:OD2	1:F:1183:LYS:NZ	1.83	1.11
1:B:1355:ASP:OD2	1:C:1183:LYS:NZ	1.92	1.02
1:A:1467:ARG:NH1	1:A:1504:ASP:OD1	2.13	0.81
1:D:1287:GLU:O	1:D:1335:HIS:NE2	2.14	0.80
1:A:1314:VAL:HG21	1:B:1309:SER:HB2	1.64	0.79
1:A:1183:LYS:NZ	1:C:1355:ASP:OD2	2.15	0.78
1:B:1314:VAL:HG21	1:C:1309:SER:HB2	1.68	0.74
1:F:1105:ARG:NH1	1:F:1429:GLU:HG3	2.04	0.72
1:F:1374:THR:HG23	1:F:1553:GLU:HG2	1.70	0.72
1:B:1284:ARG:HH21	1:B:1287:GLU:HG3	1.54	0.72
1:A:1092:SER:HB2	1:C:1090:TRP:HB2	1.73	0.70
1:A:1309:SER:HB2	1:C:1314:VAL:HG21	1.73	0.70
1:A:1390:ASP:OD1	1:A:1392:THR:OG1	2.11	0.68
1:E:1287:GLU:O	1:E:1335:HIS:NE2	2.24	0.68
1:D:1309:SER:HB2	1:F:1314:VAL:HG21	1.75	0.67
1:B:1390:ASP:OD1	1:B:1392:THR:OG1	2.12	0.67
1:B:1315:PRO:HD3	1:B:1380:SER:HB3	1.77	0.66
1:E:1094:GLU:OE2	1:E:1096:ARG:NH2	2.28	0.66
1:F:1390:ASP:OD1	1:F:1392:THR:OG1	2.14	0.66
1:C:1374:THR:HG23	1:C:1553:GLU:HG2	1.78	0.66
1:D:1374:THR:HG23	1:D:1553:GLU:HG2	1.78	0.65
1:E:1374:THR:HG23	1:E:1553:GLU:HG2	1.76	0.65
1:B:1096:ARG:HH11	1:B:1101:LEU:HD11	1.62	0.65
1:C:1390:ASP:OD1	1:C:1392:THR:OG1	2.15	0.65
1:D:1183:LYS:NZ	1:F:1355:ASP:OD2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1284:ARG:HH21	1:E:1287:GLU:HG3	1.62	0.64
1:E:1314:VAL:HG21	1:F:1309:SER:HB2	1.79	0.64
1:D:1314:VAL:HG21	1:E:1309:SER:HB2	1.79	0.64
1:D:1390:ASP:OD1	1:D:1392:THR:OG1	2.16	0.64
1:D:1494:LEU:HD22	1:D:1505:SER:HB3	1.80	0.64
1:E:1286:GLU:HG2	1:E:1289:PHE:HB2	1.79	0.63
1:D:1289:PHE:HE2	1:D:1331:LYS:HD3	1.63	0.63
1:C:1315:PRO:HD3	1:C:1380:SER:HB3	1.79	0.63
1:A:1090:TRP:HB2	1:B:1092:SER:HB2	1.81	0.62
1:E:1494:LEU:HD22	1:E:1505:SER:HB3	1.80	0.62
1:A:1508:LYS:NZ	1:A:1508:LYS:HB3	2.15	0.62
1:F:1356:LEU:HD22	1:F:1370:TYR:HD2	1.66	0.61
1:F:1494:LEU:HD22	1:F:1505:SER:HB3	1.83	0.60
1:E:1474:ASP:N	1:E:1474:ASP:OD1	2.35	0.60
1:A:1356:LEU:HD22	1:A:1370:TYR:HD1	1.66	0.60
1:B:1374:THR:HG23	1:B:1553:GLU:HG2	1.83	0.60
1:B:1497:ARG:NH1	1:B:1499:LEU:O	2.35	0.59
1:A:1060:THR:HB	1:A:1075:SER:HB3	1.85	0.59
1:E:1390:ASP:OD1	1:E:1392:THR:OG1	2.21	0.59
1:F:1474:ASP:OD1	1:F:1474:ASP:N	2.37	0.58
1:F:1354:CYS:HA	1:F:1371:THR:O	2.03	0.58
1:A:1315:PRO:HD3	1:A:1380:SER:HB3	1.85	0.58
1:F:1221:PHE:HA	1:F:1280:THR:O	2.03	0.58
1:E:1154:ASP:OD2	1:E:1217:THR:HB	2.04	0.57
1:D:1315:PRO:HD3	1:D:1380:SER:HB3	1.86	0.57
1:C:1356:LEU:HD22	1:C:1370:TYR:HD1	1.69	0.56
1:E:1447:PHE:HB3	1:E:1538:LYS:HD2	1.86	0.56
1:E:1448:ALA:HB3	1:E:1467:ARG:HB3	1.87	0.56
1:D:1284:ARG:NH1	1:D:1287:GLU:HB2	2.20	0.56
1:E:1322:HIS:HB3	1:E:1407:ASP:OD2	2.06	0.56
1:F:1465:LYS:HD3	1:F:1504:ASP:OD2	2.06	0.56
1:D:1356:LEU:HD22	1:D:1370:TYR:HD2	1.71	0.55
1:D:1221:PHE:HB3	1:D:1281:LEU:HD23	1.88	0.55
1:B:1062:LEU:HD21	1:B:1244:ARG:HH11	1.71	0.55
2:B:1602:NAG:H3	2:B:1602:NAG:H83	1.89	0.55
1:D:1355:ASP:OD2	1:E:1183:LYS:NZ	2.34	0.54
1:B:1262:ILE:HD13	1:B:1428:VAL:HG22	1.88	0.54
1:F:1251:ALA:HB2	1:F:1266:GLU:HB3	1.89	0.54
1:F:1308:GLN:H	1:F:1319:GLN:HE22	1.56	0.54
1:E:1251:ALA:HB2	1:E:1266:GLU:HB3	1.89	0.54
1:E:1315:PRO:HD3	1:E:1380:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1098:ASN:HD21	1:E:1099:LYS:HE2	1.72	0.54
1:C:1445:LEU:HB2	1:C:1531:CYS:SG	2.48	0.53
1:C:1336:LEU:HD13	1:C:1339:LYS:HD2	1.91	0.53
1:F:1194:ASN:ND2	1:F:1200:GLY:O	2.42	0.53
1:C:1288:GLY:O	1:C:1333:ASN:HA	2.09	0.53
1:D:1251:ALA:HB2	1:D:1266:GLU:HB3	1.90	0.53
1:D:1561:LYS:O	2:D:1601:NAG:H83	2.09	0.53
1:E:1131:LYS:HE2	1:E:1433:MET:HE1	1.90	0.53
1:B:1194:ASN:ND2	1:B:1200:GLY:O	2.41	0.53
1:C:1221:PHE:HB3	1:C:1281:LEU:HD23	1.91	0.53
1:D:1154:ASP:OD2	1:D:1217:THR:HB	2.08	0.52
1:E:1469:HIS:CE1	1:E:1499:LEU:HD23	2.44	0.52
1:B:1154:ASP:OD2	1:B:1217:THR:HB	2.10	0.52
1:A:1194:ASN:ND2	1:A:1200:GLY:O	2.43	0.52
1:D:1372:GLY:C	1:D:1555:LYS:HD2	2.36	0.51
1:D:1183:LYS:HD3	1:D:1356:LEU:HB2	1.92	0.51
1:F:1364:ASP:OD1	1:F:1365:TRP:N	2.42	0.51
1:B:1096:ARG:HH11	1:B:1101:LEU:CD1	2.22	0.51
1:F:1392:THR:HA	1:F:1397:PHE:HE2	1.76	0.51
1:B:1182:HIS:ND1	1:B:1184:GLU:OE2	2.44	0.50
1:D:1221:PHE:HA	1:D:1280:THR:O	2.11	0.50
1:F:1348:TRP:CH2	1:F:1350:SER:HB2	2.47	0.50
1:C:1230:LYS:NZ	1:C:1250:GLU:OE2	2.33	0.50
1:E:1359:TYR:CG	1:F:1186:PRO:HD2	2.47	0.50
1:F:1390:ASP:OD2	1:F:1393:LYS:HE3	2.12	0.49
1:F:1221:PHE:HB3	1:F:1281:LEU:HD23	1.93	0.49
1:F:1124:VAL:HA	1:F:1434:GLU:OE2	2.13	0.49
1:B:1139:ASP:OD1	1:B:1416:ARG:NH1	2.44	0.49
1:C:1155:ARG:NH2	1:C:1317:ASP:OD2	2.45	0.49
1:C:1345:ASN:OD1	1:C:1345:ASN:N	2.46	0.49
1:C:1348:TRP:CH2	1:C:1350:SER:HB2	2.47	0.48
1:A:1064:ILE:HD12	1:A:1138:MET:HE1	1.94	0.48
1:B:1221:PHE:HB3	1:B:1281:LEU:HD23	1.94	0.48
1:F:1172:ARG:HB3	1:F:1175:CYS:HB2	1.96	0.48
1:E:1356:LEU:HD22	1:E:1370:TYR:HD2	1.78	0.48
1:C:1128:SER:OG	1:C:1129:GLU:N	2.47	0.48
1:D:1203:THR:OG1	1:D:1204:GLY:N	2.47	0.48
1:B:1068:TRP:HB2	1:B:1398:HIS:HB3	1.96	0.47
1:C:1203:THR:OG1	1:C:1204:GLY:N	2.46	0.47
1:F:1132:LEU:HD11	1:F:1438:LYS:HD2	1.96	0.47
1:F:1315:PRO:HD3	1:F:1380:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1203:THR:OG1	1:B:1204:GLY:N	2.47	0.47
1:E:1221:PHE:HA	1:E:1280:THR:O	2.14	0.47
1:F:1319:GLN:OE1	1:F:1321:TYR:OH	2.22	0.47
1:D:1322:HIS:NE2	1:F:1549:SER:OG	2.41	0.47
1:B:1068:TRP:NE1	1:B:1071:ILE:HD11	2.29	0.47
1:A:1348:TRP:CH2	1:A:1350:SER:HB2	2.50	0.47
1:A:1412:ASP:OD2	1:A:1414:LYS:HE2	2.14	0.47
1:B:1090:TRP:HB2	1:C:1092:SER:HB2	1.96	0.47
1:D:1442:ILE:HD12	1:D:1527:HIS:HB2	1.97	0.47
1:E:1203:THR:OG1	1:E:1204:GLY:N	2.47	0.47
1:B:1466:VAL:HG11	1:B:1494:LEU:HD13	1.96	0.46
1:E:1497:ARG:HD2	1:E:1502:GLY:HA2	1.97	0.46
1:F:1254:ARG:HG2	1:F:1263:THR:HG23	1.97	0.46
1:E:1138:MET:HE2	1:E:1234:ILE:HG21	1.98	0.46
1:F:1203:THR:OG1	1:F:1204:GLY:N	2.48	0.46
1:A:1400:LYS:HA	1:A:1412:ASP:O	2.16	0.46
1:B:1348:TRP:CH2	1:B:1350:SER:HB2	2.50	0.46
1:C:1138:MET:HE2	1:C:1234:ILE:HG21	1.98	0.46
1:F:1153:GLY:HA3	1:F:1216:PHE:HB3	1.98	0.46
1:D:1447:PHE:HB3	1:D:1538:LYS:HD2	1.98	0.45
1:C:1221:PHE:HA	1:C:1280:THR:O	2.17	0.45
1:D:1356:LEU:HD22	1:D:1370:TYR:CD2	2.52	0.45
1:B:1067:PRO:HD3	1:B:1248:LEU:HD11	1.98	0.45
1:C:1372:GLY:C	1:C:1555:LYS:HD2	2.41	0.45
1:E:1348:TRP:CH2	1:E:1350:SER:HB2	2.51	0.45
1:A:1186:PRO:HD2	1:C:1359:TYR:CG	2.51	0.45
1:A:1356:LEU:HD22	1:A:1370:TYR:CD1	2.51	0.45
1:C:1354:CYS:HA	1:C:1371:THR:O	2.17	0.45
1:F:1131:LYS:HD3	1:F:1433:MET:HE1	1.99	0.45
1:A:1251:ALA:HB2	1:A:1266:GLU:HB3	1.99	0.45
1:E:1288:GLY:HA3	1:E:1335:HIS:CD2	2.52	0.45
1:A:1364:ASP:OD1	1:A:1365:TRP:N	2.44	0.45
1:F:1155:ARG:NH2	1:F:1317:ASP:OD2	2.44	0.45
1:A:1494:LEU:HD22	1:A:1505:SER:HB3	1.98	0.45
1:B:1064:ILE:HD12	1:B:1138:MET:HE1	1.99	0.45
1:B:1471:ASP:O	1:B:1498:LYS:HE2	2.16	0.45
1:F:1356:LEU:HD22	1:F:1370:TYR:CD2	2.48	0.45
1:B:1183:LYS:HD3	1:B:1185:TRP:CZ2	2.52	0.44
1:A:1466:VAL:HG11	1:A:1494:LEU:HD13	1.98	0.44
1:D:1092:SER:HB3	1:F:1090:TRP:HB2	1.98	0.44
1:E:1364:ASP:OD1	1:E:1365:TRP:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1124:VAL:HG12	1:E:1125:GLU:HG2	1.99	0.44
1:A:1182:HIS:ND1	1:A:1184:GLU:OE2	2.49	0.44
1:B:1364:ASP:OD1	1:B:1365:TRP:N	2.48	0.44
1:D:1345:ASN:OD1	1:D:1345:ASN:N	2.50	0.44
1:A:1203:THR:OG1	1:A:1204:GLY:N	2.49	0.44
1:A:1445:LEU:HB2	1:A:1531:CYS:SG	2.58	0.44
1:D:1284:ARG:HH11	1:D:1287:GLU:HB2	1.82	0.44
1:E:1172:ARG:NH2	1:E:1177:SER:O	2.42	0.44
1:A:1189:ARG:O	1:A:1202:GLY:N	2.42	0.44
1:B:1281:LEU:HB2	1:B:1297:LYS:HB2	2.00	0.43
1:E:1356:LEU:HD22	1:E:1370:TYR:CD2	2.54	0.43
1:D:1364:ASP:OD1	1:D:1365:TRP:N	2.50	0.43
1:B:1096:ARG:HD3	1:B:1101:LEU:HD12	2.00	0.43
1:E:1336:LEU:HD13	1:E:1339:LYS:HD2	2.00	0.43
1:D:1113:GLU:OE2	1:D:1493:SER:HB3	2.18	0.43
1:D:1139:ASP:OD1	1:D:1416:ARG:NH2	2.52	0.43
1:D:1348:TRP:CH2	1:D:1350:SER:HB2	2.54	0.43
1:D:1124:VAL:HG13	1:E:1095:HIS:O	2.19	0.43
1:F:1336:LEU:HD13	1:F:1339:LYS:HD2	2.01	0.43
1:E:1308:GLN:H	1:E:1319:GLN:HE22	1.66	0.43
1:F:1219:TYR:CE1	1:F:1385:LEU:HD11	2.54	0.43
1:A:1508:LYS:HB3	1:A:1508:LYS:HZ2	1.83	0.42
1:D:1308:GLN:H	1:D:1319:GLN:HE22	1.65	0.42
1:E:1345:ASN:OD1	1:E:1345:ASN:N	2.52	0.42
1:D:1077:TYR:HD2	1:D:1244:ARG:NH1	2.17	0.42
1:C:1356:LEU:HD22	1:C:1370:TYR:CD1	2.51	0.42
1:A:1143:MET:HE1	1:A:1414:LYS:HD3	2.01	0.42
1:B:1254:ARG:HA	1:B:1262:ILE:O	2.19	0.42
1:A:1374:THR:HG23	1:A:1553:GLU:HG2	2.00	0.42
1:A:1354:CYS:HA	1:A:1371:THR:O	2.19	0.42
1:B:1221:PHE:HA	1:B:1280:THR:O	2.20	0.42
1:E:1162:LYS:HB2	1:E:1207:CYS:HB3	2.02	0.42
1:E:1448:ALA:N	1:E:1467:ARG:O	2.46	0.42
1:B:1325:ASN:ND2	1:B:1341:GLU:HG2	2.35	0.42
1:E:1433:MET:HB3	1:E:1433:MET:HE2	1.87	0.42
1:F:1138:MET:HE2	1:F:1234:ILE:HG21	2.01	0.42
1:D:1092:SER:CB	1:F:1090:TRP:HB2	2.50	0.41
1:C:1112:LEU:HD11	1:C:1267:PRO:HB3	2.03	0.41
1:F:1400:LYS:HA	1:F:1412:ASP:O	2.20	0.41
1:B:1494:LEU:HD22	1:B:1505:SER:HB3	2.02	0.41
1:D:1445:LEU:HD23	1:D:1445:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:MET:HE2	1:B:1234:ILE:HG21	2.03	0.41
1:B:1480:VAL:HG13	1:B:1520:PHE:HB3	2.01	0.41
1:C:1095:HIS:NE2	1:C:1097:GLY:O	2.52	0.41
1:C:1442:ILE:HA	1:C:1472:GLU:O	2.20	0.41
1:D:1293:MET:HE2	1:D:1330:ASP:HA	2.02	0.41
1:C:1364:ASP:OD1	1:C:1365:TRP:N	2.44	0.41
1:C:1433:MET:HE2	1:C:1433:MET:HB3	1.95	0.41
1:A:1282:HIS:HB3	1:A:1291:ASP:O	2.21	0.41
1:D:1293:MET:HG2	1:D:1330:ASP:HB3	2.03	0.41
1:E:1221:PHE:HB3	1:E:1281:LEU:HD23	2.02	0.41
1:E:1282:HIS:HB3	1:E:1291:ASP:O	2.20	0.41
1:D:1182:HIS:ND1	1:D:1184:GLU:OE2	2.48	0.40
1:D:1242:GLN:HB3	1:D:1257:LEU:HD21	2.03	0.40
1:A:1462:ILE:O	1:A:1508:LYS:HA	2.22	0.40
1:B:1282:HIS:HB3	1:B:1291:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/540 (93%)	490 (97%)	13 (3%)	0	100	100
1	B	503/540 (93%)	490 (97%)	12 (2%)	1 (0%)	43	73
1	C	494/540 (92%)	481 (97%)	12 (2%)	1 (0%)	43	73
1	D	495/540 (92%)	481 (97%)	13 (3%)	1 (0%)	43	73
1	E	495/540 (92%)	479 (97%)	14 (3%)	2 (0%)	30	62
1	F	495/540 (92%)	482 (97%)	13 (3%)	0	100	100
All	All	2985/3240 (92%)	2903 (97%)	77 (3%)	5 (0%)	43	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1097	GLY
1	E	1097	GLY
1	B	1097	GLY
1	D	1554	HIS
1	E	1504	ASP

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	448/479 (94%)	436 (97%)	12 (3%)	39	70
1	B	448/479 (94%)	440 (98%)	8 (2%)	51	76
1	C	441/479 (92%)	434 (98%)	7 (2%)	55	78
1	D	442/479 (92%)	432 (98%)	10 (2%)	44	72
1	E	442/479 (92%)	433 (98%)	9 (2%)	48	75
1	F	442/479 (92%)	435 (98%)	7 (2%)	55	78
All	All	2663/2874 (93%)	2610 (98%)	53 (2%)	48	75

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1098	ASN
1	A	1100	ILE
1	A	1102	VAL
1	A	1166	THR
1	A	1216	PHE
1	A	1226	VAL
1	A	1304	VAL
1	A	1332	VAL
1	A	1453	THR
1	A	1491	SER
1	A	1516	THR
1	A	1523	VAL
1	B	1081	VAL
1	B	1100	ILE

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Mol	Chain	Res	Type
1	B	1216	PHE
1	B	1226	VAL
1	B	1304	VAL
1	B	1491	SER
1	B	1503	THR
1	B	1523	VAL
1	C	1081	VAL
1	C	1166	THR
1	C	1216	PHE
1	C	1304	VAL
1	C	1491	SER
1	C	1503	THR
1	C	1516	THR
1	D	1100	ILE
1	D	1101	LEU
1	D	1102	VAL
1	D	1166	THR
1	D	1216	PHE
1	D	1304	VAL
1	D	1453	THR
1	D	1499	LEU
1	D	1516	THR
1	D	1523	VAL
1	E	1102	VAL
1	E	1166	THR
1	E	1216	PHE
1	E	1226	VAL
1	E	1304	VAL
1	E	1453	THR
1	E	1499	LEU
1	E	1504	ASP
1	E	1516	THR
1	F	1166	THR
1	F	1193	CYS
1	F	1216	PHE
1	F	1226	VAL
1	F	1304	VAL
1	F	1491	SER
1	F	1516	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1378	HIS
1	A	1398	HIS
1	C	1361	ASN
1	C	1436	HIS
1	D	1405	HIS
1	D	1469	HIS
1	E	1376	HIS
1	E	1396	HIS
1	E	1405	HIS
1	F	1256	ASN
1	F	1361	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\# Z > 2$
2	NAG	C	1601	1	14,14,15	0.47	0	17,19,21	0.65	1 (5%)
2	NAG	B	1602	1	14,14,15	0.40	0	17,19,21	1.34	2 (11%)
2	NAG	D	1601	1	14,14,15	0.54	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	F	1601	1	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	C	1602	1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	E	1601	1	14,14,15	0.17	0	17,19,21	0.52	0
2	NAG	A	1602	1	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	A	1601	1	14,14,15	0.27	0	17,19,21	0.45	0
2	NAG	B	1601	1	14,14,15	0.19	0	17,19,21	0.39	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
2	NAG	C	1601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1602	1	-	6/6/23/26	0/1/1/1
2	NAG	D	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	F	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1602	1	-	4/6/23/26	0/1/1/1
2	NAG	E	1601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1602	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1601	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1602	NAG	C2-N2-C7	4.61	129.08	122.90
2	D	1601	NAG	C1-O5-C5	2.54	115.59	112.19
2	C	1601	NAG	C1-O5-C5	2.26	115.22	112.19
2	B	1602	NAG	C1-C2-N2	2.22	113.92	110.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1602	NAG	O5-C5-C6-O6
2	B	1602	NAG	C4-C5-C6-O6
2	A	1601	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	1601	NAG	O7-C7-N2-C2
2	B	1602	NAG	C8-C7-N2-C2
2	B	1602	NAG	O7-C7-N2-C2
2	C	1602	NAG	C8-C7-N2-C2
2	C	1602	NAG	O7-C7-N2-C2
2	E	1601	NAG	C8-C7-N2-C2
2	E	1601	NAG	O7-C7-N2-C2
2	F	1601	NAG	C8-C7-N2-C2
2	F	1601	NAG	O7-C7-N2-C2
2	C	1602	NAG	O5-C5-C6-O6
2	C	1602	NAG	C4-C5-C6-O6
2	B	1601	NAG	C4-C5-C6-O6
2	B	1601	NAG	O5-C5-C6-O6
2	A	1602	NAG	C1-C2-N2-C7
2	A	1601	NAG	C4-C5-C6-O6
2	D	1601	NAG	C3-C2-N2-C7
2	B	1602	NAG	C1-C2-N2-C7
2	D	1601	NAG	C1-C2-N2-C7
2	A	1602	NAG	C3-C2-N2-C7
2	B	1602	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1602	NAG	1	0
2	D	1601	NAG	1	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	505/540 (93%)	-0.07	1 (0%) 91 85	42, 69, 124, 171	0
1	B	505/540 (93%)	-0.09	1 (0%) 91 85	40, 66, 123, 182	0
1	C	498/540 (92%)	-0.01	5 (1%) 79 63	43, 71, 131, 191	0
1	D	499/540 (92%)	0.14	3 (0%) 85 72	68, 106, 158, 235	0
1	E	499/540 (92%)	0.19	3 (0%) 85 72	79, 114, 170, 230	0
1	F	499/540 (92%)	0.14	2 (0%) 88 79	70, 101, 157, 191	0
All	All	3005/3240 (92%)	0.05	15 (0%) 87 75	40, 90, 151, 235	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1107	GLU	3.9
1	E	1191	HIS	3.4
1	F	1334	GLY	3.0
1	A	1355	ASP	2.7
1	C	1346	THR	2.6
1	D	1191	HIS	2.5
1	D	1069	GLY	2.4
1	B	1555	LYS	2.3
1	E	1352	ASP	2.2
1	C	1337	ILE	2.2
1	D	1119	SER	2.2
1	F	1082	SER	2.2
1	C	1061	SER	2.1
1	C	1558	ILE	2.1
1	C	1065	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	A	1601	14/15	0.12	0.14	134,144,150,151	0
2	NAG	B	1601	14/15	0.26	0.13	137,145,152,153	0
2	NAG	E	1601	14/15	0.26	0.11	163,174,178,183	0
2	NAG	F	1601	14/15	0.33	0.12	145,165,170,170	0
2	NAG	C	1602	14/15	0.45	0.10	139,157,162,163	0
2	NAG	A	1602	14/15	0.48	0.15	128,138,145,145	0
2	NAG	B	1602	14/15	0.54	0.12	124,135,140,140	0
2	NAG	D	1601	14/15	0.57	0.11	166,191,219,224	0
2	NAG	C	1601	14/15	0.59	0.12	133,143,156,157	0
3	CL	A	1604	1/1	0.78	0.10	87,87,87,87	0
3	CL	A	1603	1/1	0.91	0.12	94,94,94,94	0
3	CL	D	1603	1/1	0.91	0.09	94,94,94,94	0
3	CL	D	1602	1/1	0.94	0.12	82,82,82,82	0
3	CL	C	1603	1/1	0.98	0.08	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.