



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 3M5N / pdb_00003m5n
Title : Crystal structure of HCV NS3/4A protease in complex with N-terminal product 4B5A
Authors : Schiffer, C.A.; Romano, K.P.
Deposited on : 2010-03-12
Resolution : 1.90 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 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

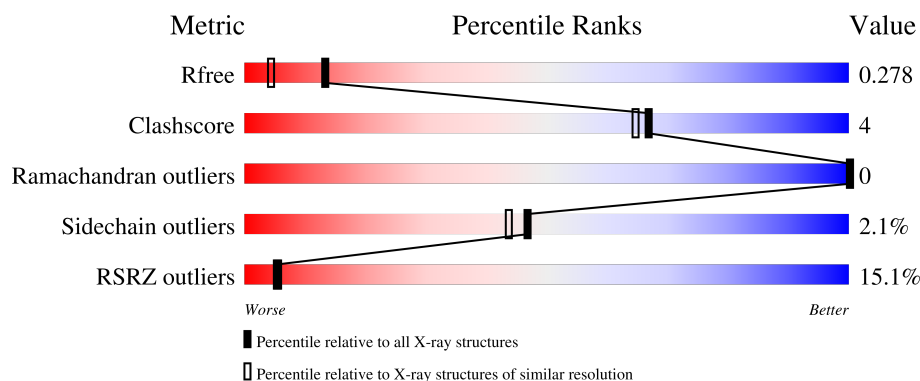
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 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	203	
1	B	203	
1	C	203	
1	D	203	
2	F	7	

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Mol	Chain	Length	Quality of chain
2	G	7	57% 86% 14%
2	H	7	57% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6372 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 NS3/4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1445	894	266	277	8			
1	B	199	Total	C	N	O	S	0	0	0
			1420	880	257	275	8			
1	C	197	Total	C	N	O	S	0	0	0
			1418	881	260	269	8			
1	D	198	Total	C	N	O	S	0	0	0
			1421	881	257	275	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	981	SER	-	expression tag	UNP A8DG50
A	982	HIS	-	expression tag	UNP A8DG50
A	983	MET	-	expression tag	UNP A8DG50
A	984	ALA	-	expression tag	UNP A8DG50
A	985	SER	-	expression tag	UNP A8DG50
A	986	MET	-	engineered mutation	UNP A8DG50
A	987	LYS	-	engineered mutation	UNP A8DG50
A	988	LYS	-	engineered mutation	UNP A8DG50
A	989	LYS	-	engineered mutation	UNP A8DG50
A	991	SER	CYS	SEE REMARK 999	UNP A8DG50
A	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
A	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
A	1001	SER	ALA	engineered mutation	UNP A8DG50
A	1002	GLY	PRO	engineered mutation	UNP A8DG50
A	1003	ASP	ILE	engineered mutation	UNP A8DG50
A	1013	GLU	LEU	engineered mutation	UNP A8DG50
A	1014	GLU	LEU	engineered mutation	UNP A8DG50
A	1017	GLN	ILE	engineered mutation	UNP A8DG50
A	1018	GLU	ILE	engineered mutation	UNP A8DG50
A	1021	GLN	LEU	engineered mutation	UNP A8DG50
A	1040	THR	ALA	engineered mutation	UNP A8DG50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	SER	CYS	engineered mutation	UNP A8DG50
A	1052	LEU	CYS	engineered mutation	UNP A8DG50
A	1072	THR	ILE	engineered mutation	UNP A8DG50
A	1086	GLN	PRO	engineered mutation	UNP A8DG50
A	1139	ALA	SER	engineered mutation	UNP A8DG50
A	1159	SER	CYS	engineered mutation	UNP A8DG50
B	981	SER	-	expression tag	UNP A8DG50
B	982	HIS	-	expression tag	UNP A8DG50
B	983	MET	-	expression tag	UNP A8DG50
B	984	ALA	-	expression tag	UNP A8DG50
B	985	SER	-	expression tag	UNP A8DG50
B	986	MET	-	engineered mutation	UNP A8DG50
B	987	LYS	-	engineered mutation	UNP A8DG50
B	988	LYS	-	engineered mutation	UNP A8DG50
B	989	LYS	-	engineered mutation	UNP A8DG50
B	991	SER	CYS	SEE REMARK 999	UNP A8DG50
B	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
B	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
B	1001	SER	ALA	engineered mutation	UNP A8DG50
B	1002	GLY	PRO	engineered mutation	UNP A8DG50
B	1003	ASP	ILE	engineered mutation	UNP A8DG50
B	1013	GLU	LEU	engineered mutation	UNP A8DG50
B	1014	GLU	LEU	engineered mutation	UNP A8DG50
B	1017	GLN	ILE	engineered mutation	UNP A8DG50
B	1018	GLU	ILE	engineered mutation	UNP A8DG50
B	1021	GLN	LEU	engineered mutation	UNP A8DG50
B	1040	THR	ALA	engineered mutation	UNP A8DG50
B	1047	SER	CYS	engineered mutation	UNP A8DG50
B	1052	LEU	CYS	engineered mutation	UNP A8DG50
B	1072	THR	ILE	engineered mutation	UNP A8DG50
B	1086	GLN	PRO	engineered mutation	UNP A8DG50
B	1139	ALA	SER	engineered mutation	UNP A8DG50
B	1159	SER	CYS	engineered mutation	UNP A8DG50
C	981	SER	-	expression tag	UNP A8DG50
C	982	HIS	-	expression tag	UNP A8DG50
C	983	MET	-	expression tag	UNP A8DG50
C	984	ALA	-	expression tag	UNP A8DG50
C	985	SER	-	expression tag	UNP A8DG50
C	986	MET	-	engineered mutation	UNP A8DG50
C	987	LYS	-	engineered mutation	UNP A8DG50
C	988	LYS	-	engineered mutation	UNP A8DG50
C	989	LYS	-	engineered mutation	UNP A8DG50

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Chain	Residue	Modelled	Actual	Comment	Reference
C	991	SER	CYS	SEE REMARK 999	UNP A8DG50
C	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
C	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
C	1001	SER	ALA	engineered mutation	UNP A8DG50
C	1002	GLY	PRO	engineered mutation	UNP A8DG50
C	1003	ASP	ILE	engineered mutation	UNP A8DG50
C	1013	GLU	LEU	engineered mutation	UNP A8DG50
C	1014	GLU	LEU	engineered mutation	UNP A8DG50
C	1017	GLN	ILE	engineered mutation	UNP A8DG50
C	1018	GLU	ILE	engineered mutation	UNP A8DG50
C	1021	GLN	LEU	engineered mutation	UNP A8DG50
C	1040	THR	ALA	engineered mutation	UNP A8DG50
C	1047	SER	CYS	engineered mutation	UNP A8DG50
C	1052	LEU	CYS	engineered mutation	UNP A8DG50
C	1072	THR	ILE	engineered mutation	UNP A8DG50
C	1086	GLN	PRO	engineered mutation	UNP A8DG50
C	1139	ALA	SER	engineered mutation	UNP A8DG50
C	1159	SER	CYS	engineered mutation	UNP A8DG50
D	981	SER	-	expression tag	UNP A8DG50
D	982	HIS	-	expression tag	UNP A8DG50
D	983	MET	-	expression tag	UNP A8DG50
D	984	ALA	-	expression tag	UNP A8DG50
D	985	SER	-	expression tag	UNP A8DG50
D	986	MET	-	engineered mutation	UNP A8DG50
D	987	LYS	-	engineered mutation	UNP A8DG50
D	988	LYS	-	engineered mutation	UNP A8DG50
D	989	LYS	-	engineered mutation	UNP A8DG50
D	991	SER	CYS	SEE REMARK 999	UNP A8DG50
D	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
D	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
D	1001	SER	ALA	engineered mutation	UNP A8DG50
D	1002	GLY	PRO	engineered mutation	UNP A8DG50
D	1003	ASP	ILE	engineered mutation	UNP A8DG50
D	1013	GLU	LEU	engineered mutation	UNP A8DG50
D	1014	GLU	LEU	engineered mutation	UNP A8DG50
D	1017	GLN	ILE	engineered mutation	UNP A8DG50
D	1018	GLU	ILE	engineered mutation	UNP A8DG50
D	1021	GLN	LEU	engineered mutation	UNP A8DG50
D	1040	THR	ALA	engineered mutation	UNP A8DG50
D	1047	SER	CYS	engineered mutation	UNP A8DG50
D	1052	LEU	CYS	engineered mutation	UNP A8DG50
D	1072	THR	ILE	engineered mutation	UNP A8DG50

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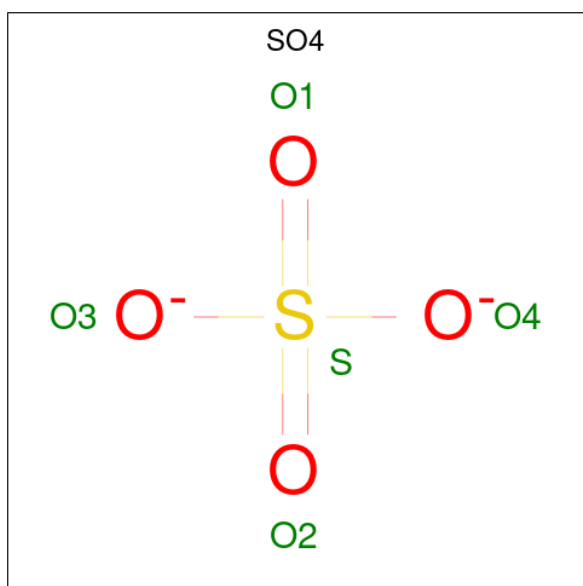
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1086	GLN	PRO	engineered mutation	UNP A8DG50
D	1139	ALA	SER	engineered mutation	UNP A8DG50
D	1159	SER	CYS	engineered mutation	UNP A8DG50

- Molecule 2 is a protein called SECTTPC peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	S	0	0	0
			49	27	7	13	2			
2	G	7	Total	C	N	O	S	0	0	0
			49	27	7	13	2			
2	H	7	Total	C	N	O	S	0	0	0
			49	27	7	13	2			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



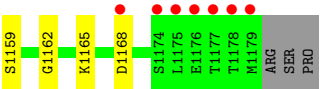
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

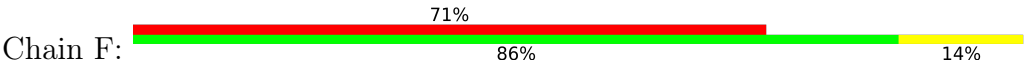
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0

- Molecule 5 is water.

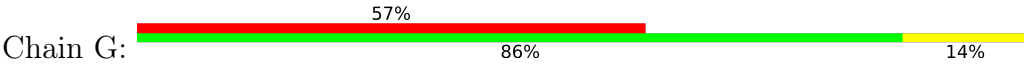
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 135	O 135	0	4
5	B	141	Total 142	O 142	0	1
5	C	103	Total 107	O 107	0	4
5	D	105	Total 107	O 107	0	2
5	F	3	Total 3	O 3	0	0
5	G	2	Total 2	O 2	0	0
5	H	1	Total 1	O 1	0	0



● Molecule 2: SECTTPC peptide



● Molecule 2: SECTTPC peptide



● Molecule 2: SECTTPC peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.31Å 58.89Å 98.27Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.90) 99.3 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.240 0.234 , 0.278	Depositor DCC
R_{free} test set	3010 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	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	6372	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.41 % 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 5.0213e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, ZN

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	0.59	0/1470	0.91	1/2001 (0.0%)
1	B	0.64	0/1445	0.94	2/1971 (0.1%)
1	C	0.54	0/1442	0.89	2/1962 (0.1%)
1	D	0.56	0/1446	0.90	0/1971
2	F	0.58	0/49	1.03	0/65
2	G	0.57	0/49	0.87	0/65
2	H	0.61	0/49	0.90	0/65
All	All	0.58	0/5950	0.91	5/8100 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1128	SER	CA-C-N	-5.57	113.96	119.92
1	C	1128	SER	C-N-CA	-5.57	113.96	119.92
1	B	1095	THR	CB-CA-C	5.22	115.94	108.68
1	B	1092	ARG	N-CA-C	-5.12	101.58	109.52
1	A	1038	THR	N-CA-C	-5.05	102.67	109.95

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	1445	0	1423	5	0
1	B	1420	0	1382	7	0
1	C	1418	0	1412	16	0
1	D	1421	0	1390	15	0
2	F	49	0	44	1	0
2	G	49	0	44	0	0
2	H	49	0	44	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	135	0	0	1	0
5	B	142	0	0	0	0
5	C	107	0	0	1	0
5	D	107	0	0	1	0
5	F	3	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
All	All	6372	0	5739	43	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 (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1132:ILE:HD11	2:F:5:THR:HB	1.61	0.82
1:C:1042:THR:HG21	1:C:1109:ARG:HH22	1.44	0.82
1:B:1042:THR:HG21	1:B:1109:ARG:HH22	1.45	0.81
1:D:1114:ILE:HD11	1:D:1134:TYR:HE2	1.52	0.75
1:C:1042:THR:CG2	1:C:1109:ARG:HH22	2.01	0.72
1:C:1160:THR:HG22	1:C:1161:ARG:HG3	1.71	0.71
1:B:1042:THR:HG22	1:B:1109:ARG:HH12	1.57	0.70
1:D:1042:THR:HG21	1:D:1109:ARG:HH22	1.59	0.67
1:C:1174:SER:HA	1:C:1177:THR:HG22	1.78	0.65
1:C:1132:ILE:HD11	1:C:1159:SER:OG	1.97	0.65
1:D:1042:THR:HG22	1:D:1109:ARG:HH12	1.64	0.62
1:C:1042:THR:HG22	1:C:1109:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1115:PRO:HB2	1:C:1127:LEU:HD22	1.86	0.57
1:C:1132:ILE:HD11	1:C:1159:SER:CB	2.35	0.56
1:C:1155:ARG:HG3	1:C:1170:ILE:HG13	1.89	0.55
1:D:1042:THR:CG2	1:D:1109:ARG:HH22	2.20	0.54
1:B:1042:THR:CG2	1:B:1109:ARG:HH22	2.18	0.52
1:A:1096:PRO:HB3	1:A:1172:VAL:HG21	1.92	0.51
1:A:1106:LEU:HD11	5:A:127:HOH:O	2.12	0.49
1:D:1132:ILE:HD12	1:D:1162:GLY:HA2	1.94	0.49
1:D:1132:ILE:HD11	1:D:1159:SER:OG	2.13	0.48
1:D:1115:PRO:HB2	1:D:1127:LEU:HD22	1.95	0.48
1:C:1114:ILE:HD11	1:C:1134:TYR:HE2	1.77	0.48
1:D:1116:VAL:HG22	1:D:1126:LEU:HD23	1.96	0.48
1:A:1115:PRO:HB2	1:A:1127:LEU:HD22	1.95	0.47
1:C:1149:HIS:ND1	5:C:486:HOH:O	2.22	0.47
1:D:1104:LEU:HD11	1:D:1118:ARG:HG3	1.97	0.47
1:B:1116:VAL:HG22	1:B:1126:LEU:HD23	1.96	0.47
1:D:1127:LEU:N	1:D:1127:LEU:CD1	2.78	0.47
1:C:1042:THR:HG21	1:C:1109:ARG:NH2	2.24	0.46
1:D:1074:MET:HE2	1:D:1075:TYR:CE2	2.51	0.46
1:C:1042:THR:CG2	1:C:1109:ARG:NH2	2.76	0.46
1:D:1114:ILE:HD11	1:D:1134:TYR:CE2	2.42	0.45
1:D:1106:LEU:HD11	5:D:90:HOH:O	2.16	0.45
1:C:1116:VAL:HG22	1:C:1126:LEU:HD23	1.99	0.45
1:A:1114:ILE:HG23	1:A:1130:ARG:NH1	2.33	0.44
1:B:1123:ARG:NE	1:B:1168:ASP:OD2	2.51	0.44
1:C:1114:ILE:HD11	1:C:1134:TYR:CE2	2.53	0.43
1:D:1123:ARG:HG2	1:D:1168:ASP:OD2	2.19	0.43
1:A:1132:ILE:HD11	1:A:1157:ALA:HB3	2.01	0.42
1:D:1036:VAL:O	1:D:1042:THR:HG23	2.21	0.41
1:C:1106:LEU:HD13	1:C:1143:LEU:HD22	2.03	0.40
1:B:1042:THR:CG2	1:B:1109:ARG:HH12	2.32	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	198/203 (98%)	197 (100%)	1 (0%)	0	100	100
1	B	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
1	C	195/203 (96%)	194 (100%)	1 (0%)	0	100	100
1	D	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
2	F	5/7 (71%)	5 (100%)	0	0	100	100
2	G	5/7 (71%)	5 (100%)	0	0	100	100
2	H	5/7 (71%)	5 (100%)	0	0	100	100
All	All	801/833 (96%)	795 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	152/164 (93%)	149 (98%)	3 (2%)	48	46
1	B	148/164 (90%)	146 (99%)	2 (1%)	59	59
1	C	149/164 (91%)	145 (97%)	4 (3%)	39	34
1	D	149/164 (91%)	146 (98%)	3 (2%)	48	46
2	F	7/7 (100%)	7 (100%)	0	100	100
2	G	7/7 (100%)	6 (86%)	1 (14%)	3	1
2	H	7/7 (100%)	7 (100%)	0	100	100
All	All	619/677 (91%)	606 (98%)	13 (2%)	47	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	GLN
1	A	1109	ARG

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Mol	Chain	Res	Type
1	A	1121	ASP
1	B	1095	THR
1	B	1117	ARG
1	C	1066	SER
1	C	1095	THR
1	C	1155	ARG
1	C	1165	LYS
1	D	1117	ARG
1	D	1127	LEU
1	D	1165	LYS
2	G	3	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	ASN
1	B	1086	GLN
1	C	1017	GLN
1	C	1027	ASN
1	C	1028	GLN
1	D	1017	GLN
1	D	1027	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	A	1	-	4,4,4	0.32	0	6,6,6	0.32	0
3	SO4	C	3	-	4,4,4	0.33	0	6,6,6	0.23	0
3	SO4	D	4	-	4,4,4	0.27	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	200/203 (98%)	0.97	29 (14%) 6 6	14, 28, 47, 64	0
1	B	199/203 (98%)	0.77	24 (12%) 8 9	13, 26, 43, 62	0
1	C	197/203 (97%)	0.98	28 (14%) 6 6	18, 30, 51, 62	0
1	D	198/203 (97%)	1.01	29 (14%) 6 6	16, 29, 49, 63	0
2	F	7/7 (100%)	2.79	5 (71%) 0 0	45, 47, 55, 55	0
2	G	7/7 (100%)	3.04	4 (57%) 0 0	48, 49, 61, 61	0
2	H	7/7 (100%)	2.06	4 (57%) 0 0	44, 45, 56, 58	0
All	All	815/833 (97%)	0.98	123 (15%) 5 5	13, 29, 50, 64	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	7	CYS	5.8
2	G	7	CYS	5.7
1	C	1177	THR	5.3
1	A	1134	TYR	5.1
1	C	1174	SER	4.8
2	G	3	CYS	4.6
1	C	1178	THR	4.0
2	G	1	SER	4.0
1	D	1177	THR	3.9
1	D	1089	GLN	3.9
1	D	1028	GLN	3.8
1	D	1086	GLN	3.8
1	A	985	SER	3.8
1	D	1176	GLU	3.8
1	D	985	SER	3.6
2	F	3	CYS	3.5
1	B	1178	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	1001	SER	3.4
1	A	1121	ASP	3.3
1	A	1100	GLY	3.3
1	A	1103	ASP	3.3
1	C	1173	GLU	3.2
1	C	1102	SER	3.2
1	D	1178	THR	3.1
1	B	986	MET	3.1
1	A	1004	THR	3.1
1	C	1098	THR	3.0
1	D	984	ALA	3.0
1	D	1179	MET	3.0
1	A	1102	SER	3.0
1	B	1120	GLY	3.0
1	B	1134	TYR	3.0
1	B	1121	ASP	3.0
1	C	1176	GLU	2.9
1	A	1040	THR	2.9
1	C	986	MET	2.9
1	C	1069	GLY	2.9
1	D	986	MET	2.9
1	B	1166	ALA	2.8
2	F	5	THR	2.8
1	B	1176	GLU	2.8
2	H	1	SER	2.7
1	A	1099	CYS	2.7
1	C	1149	HIS	2.7
1	A	1098	THR	2.7
1	B	1040	THR	2.7
1	B	1177	THR	2.7
1	D	1087	ALA	2.7
1	D	1102	SER	2.7
1	D	982	HIS	2.7
1	A	986	MET	2.6
1	D	1175	LEU	2.6
1	C	1090	GLY	2.6
1	A	1018	GLU	2.6
1	B	987	LYS	2.6
1	C	1099	CYS	2.5
1	B	1158	VAL	2.5
1	A	1028	GLN	2.5
1	C	1028	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	7	CYS	2.5
1	B	981	SER	2.5
1	A	1095	THR	2.5
2	H	6	PRO	2.5
1	A	981	SER	2.4
1	D	987	LYS	2.4
1	C	1040	THR	2.4
1	A	1180	ARG	2.4
1	D	1101	SER	2.4
1	A	1127	LEU	2.4
1	A	1178	THR	2.4
1	D	1120	GLY	2.4
1	A	1128	SER	2.4
1	B	1133	SER	2.4
1	D	1091	SER	2.4
1	D	1127	LEU	2.3
2	F	4	THR	2.3
1	C	984	ALA	2.3
1	A	1012	GLY	2.3
1	B	1003	ASP	2.3
1	C	1161	ARG	2.3
1	C	1175	LEU	2.3
1	D	1039	ALA	2.3
1	D	1090	GLY	2.3
1	C	1014	GLU	2.3
1	A	1089	GLN	2.3
1	D	1013	GLU	2.3
1	B	1028	GLN	2.3
1	D	1040	THR	2.3
1	D	1174	SER	2.2
1	C	1179	MET	2.2
1	D	1021	GLN	2.2
1	A	1101	SER	2.2
1	A	1039	ALA	2.2
1	D	1114	ILE	2.2
1	C	1168	ASP	2.2
1	D	1100	GLY	2.2
1	C	1089	GLN	2.1
1	B	1004	THR	2.1
1	C	1160	THR	2.1
1	D	1168	ASP	2.1
1	A	1001	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	990	GLY	2.1
1	B	988	LYS	2.1
1	B	991	SER	2.1
1	D	1029	VAL	2.1
1	C	1097	CYS	2.1
1	A	1014	GLU	2.1
1	C	1100	GLY	2.1
1	B	1179	MET	2.1
1	A	1097	CYS	2.1
1	B	1102	SER	2.0
1	A	1179	MET	2.0
1	A	1025	ASP	2.0
1	C	1121	ASP	2.0
1	A	1013	GLU	2.0
1	B	989	LYS	2.0
2	F	1	SER	2.0
1	B	982	HIS	2.0
1	B	1098	THR	2.0
1	C	1086	GLN	2.0
2	G	4	THR	2.0
2	H	5	THR	2.0
1	B	1119	ARG	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
3	SO4	D	4	5/5	0.91	0.16	40,41,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	3	5/5	0.93	0.21	38,40,42,45	0
3	SO4	A	1	5/5	0.94	0.15	36,36,39,39	0
4	ZN	A	1181	1/1	0.94	0.07	34,34,34,34	0
3	SO4	B	2	5/5	0.95	0.14	37,40,42,42	0
4	ZN	D	1181	1/1	0.96	0.06	33,33,33,33	0
4	ZN	C	1181	1/1	0.97	0.06	41,41,41,41	0
4	ZN	B	1181	1/1	0.98	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.