



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:59 PM UTC

PDB ID : 5FPS / pdb_00005fps
Title : Structure of hepatitis C virus (HCV) full-length NS3 complex with small-molecule ligand 3-aminobenzene-1,2-dicarboxylic acid (AT1246) in an alternate binding site.
Authors : Jhoti, H.; Ludlow, R.F.; Saini, H.K.; Tickle, I.J.; Verdonk, M.; Williams, P.A.
Deposited on : 2015-12-02
Resolution : 2.68 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

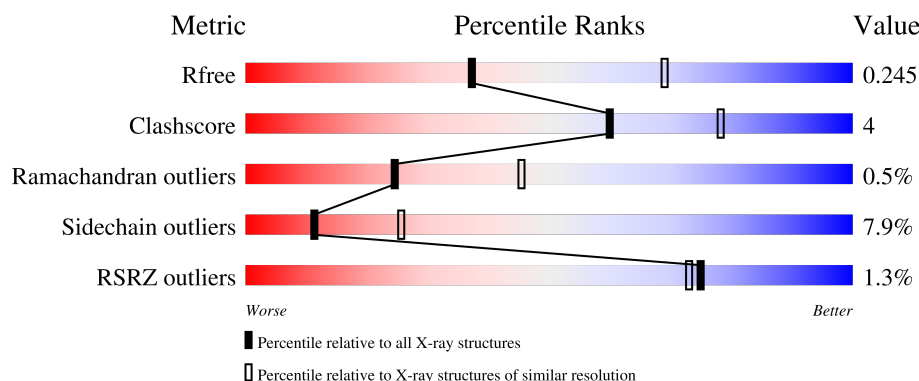
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

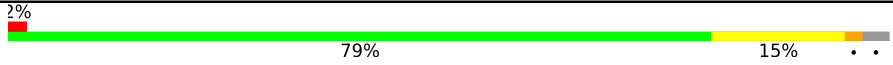
The reported resolution of this entry is 2.68 Å.

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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	666	
1	B	666	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10116 atoms, of which 10 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 HEPATITIS C VIRUS FULL-LENGTH NS3 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	0	0
			4701	2965	793	913	30			
1	B	642	Total	C	N	O	S	0	0	0
			4692	2972	792	898	30			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	684	MET	-	initiating methionine	UNP P26663
A	685	GLY	-	expression tag	UNP P26663
A	686	SER	-	expression tag	UNP P26663
A	687	SER	-	expression tag	UNP P26663
A	688	HIS	-	expression tag	UNP P26663
A	689	HIS	-	expression tag	UNP P26663
A	690	HIS	-	expression tag	UNP P26663
A	691	HIS	-	expression tag	UNP P26663
A	692	HIS	-	expression tag	UNP P26663
A	693	HIS	-	expression tag	UNP P26663
A	694	SER	-	expression tag	UNP P26663
A	695	SER	-	expression tag	UNP P26663
A	696	GLY	-	expression tag	UNP P26663
A	697	LEU	-	expression tag	UNP P26663
A	698	VAL	-	expression tag	UNP P26663
A	699	PRO	-	expression tag	UNP P26663
A	700	ARG	-	expression tag	UNP P26663
A	701	GLY	-	expression tag	UNP P26663
A	702	SER	-	expression tag	UNP P26663
A	703	HIS	-	expression tag	UNP P26663
A	704	MET	-	expression tag	UNP P26663
A	705	GLY	-	expression tag	UNP P26663
A	706	SER	-	expression tag	UNP P26663
A	707	VAL	-	expression tag	UNP P26663
A	708	VAL	-	expression tag	UNP P26663

Continued on next page...

Continued from previous page...

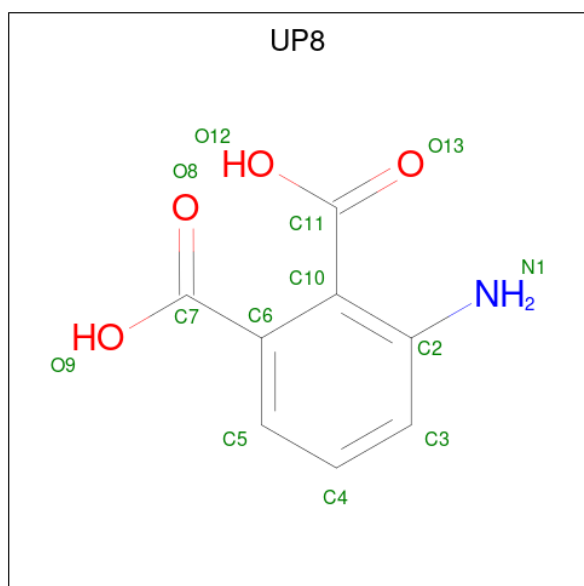
Chain	Residue	Modelled	Actual	Comment	Reference
A	709	ILE	-	expression tag	UNP P26663
A	710	VAL	-	expression tag	UNP P26663
A	711	GLY	-	expression tag	UNP P26663
A	712	ARG	-	expression tag	UNP P26663
A	713	ILE	-	expression tag	UNP P26663
A	714	ILE	-	expression tag	UNP P26663
A	715	LEU	-	expression tag	UNP P26663
A	716	SER	-	expression tag	UNP P26663
A	717	GLY	-	expression tag	UNP P26663
A	718	SER	-	expression tag	UNP P26663
A	719	GLY	-	expression tag	UNP P26663
A	720	SER	-	expression tag	UNP P26663
A	66	GLY	ALA	conflict	UNP P26663
A	86	GLN	PRO	conflict	UNP P26663
A	87	ALA	LYS	conflict	UNP P26663
A	147	SER	PHE	conflict	UNP P26663
B	684	MET	-	initiating methionine	UNP P26663
B	685	GLY	-	expression tag	UNP P26663
B	686	SER	-	expression tag	UNP P26663
B	687	SER	-	expression tag	UNP P26663
B	688	HIS	-	expression tag	UNP P26663
B	689	HIS	-	expression tag	UNP P26663
B	690	HIS	-	expression tag	UNP P26663
B	691	HIS	-	expression tag	UNP P26663
B	692	HIS	-	expression tag	UNP P26663
B	693	HIS	-	expression tag	UNP P26663
B	694	SER	-	expression tag	UNP P26663
B	695	SER	-	expression tag	UNP P26663
B	696	GLY	-	expression tag	UNP P26663
B	697	LEU	-	expression tag	UNP P26663
B	698	VAL	-	expression tag	UNP P26663
B	699	PRO	-	expression tag	UNP P26663
B	700	ARG	-	expression tag	UNP P26663
B	701	GLY	-	expression tag	UNP P26663
B	702	SER	-	expression tag	UNP P26663
B	703	HIS	-	expression tag	UNP P26663
B	704	MET	-	expression tag	UNP P26663
B	705	GLY	-	expression tag	UNP P26663
B	706	SER	-	expression tag	UNP P26663
B	707	VAL	-	expression tag	UNP P26663
B	708	VAL	-	expression tag	UNP P26663
B	709	ILE	-	expression tag	UNP P26663

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	710	VAL	-	expression tag	UNP P26663
B	711	GLY	-	expression tag	UNP P26663
B	712	ARG	-	expression tag	UNP P26663
B	713	ILE	-	expression tag	UNP P26663
B	714	ILE	-	expression tag	UNP P26663
B	715	LEU	-	expression tag	UNP P26663
B	716	SER	-	expression tag	UNP P26663
B	717	GLY	-	expression tag	UNP P26663
B	718	SER	-	expression tag	UNP P26663
B	719	GLY	-	expression tag	UNP P26663
B	720	SER	-	expression tag	UNP P26663
B	66	GLY	ALA	conflict	UNP P26663
B	86	GLN	PRO	conflict	UNP P26663
B	87	ALA	LYS	conflict	UNP P26663
B	147	SER	PHE	conflict	UNP P26663

- Molecule 2 is 3-AMINOBENZENE-1,2-DICARBOXYLIC ACID (CCD ID: UP8) (formula: $C_8H_7NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			18	8	5	1	4		
2	B	1	Total	C	H	N	O	0	0
			18	8	5	1	4		

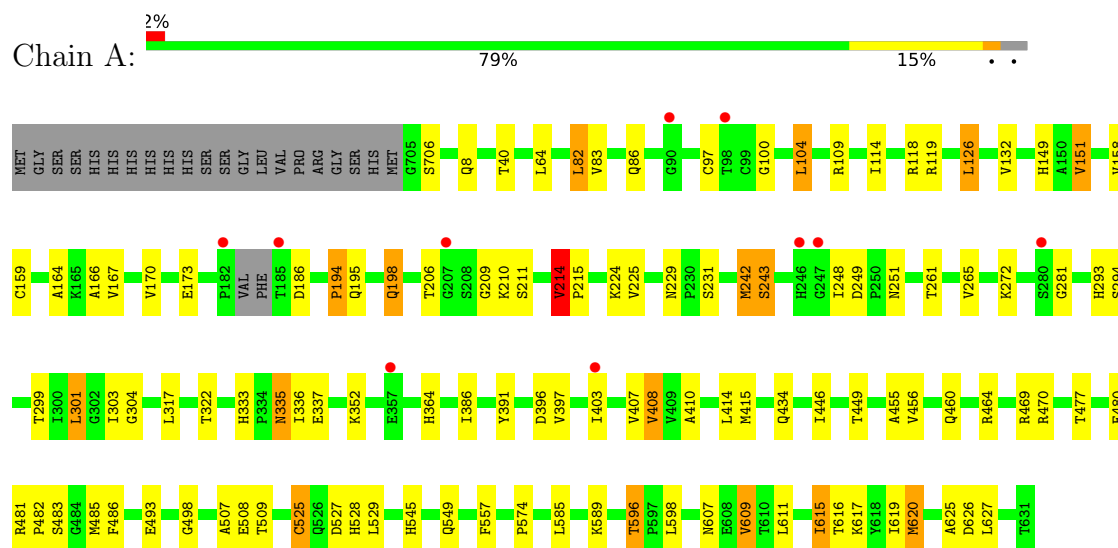
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	347	Total 347	O 347	0	0
3	B	340	Total 340	O 340	0	0

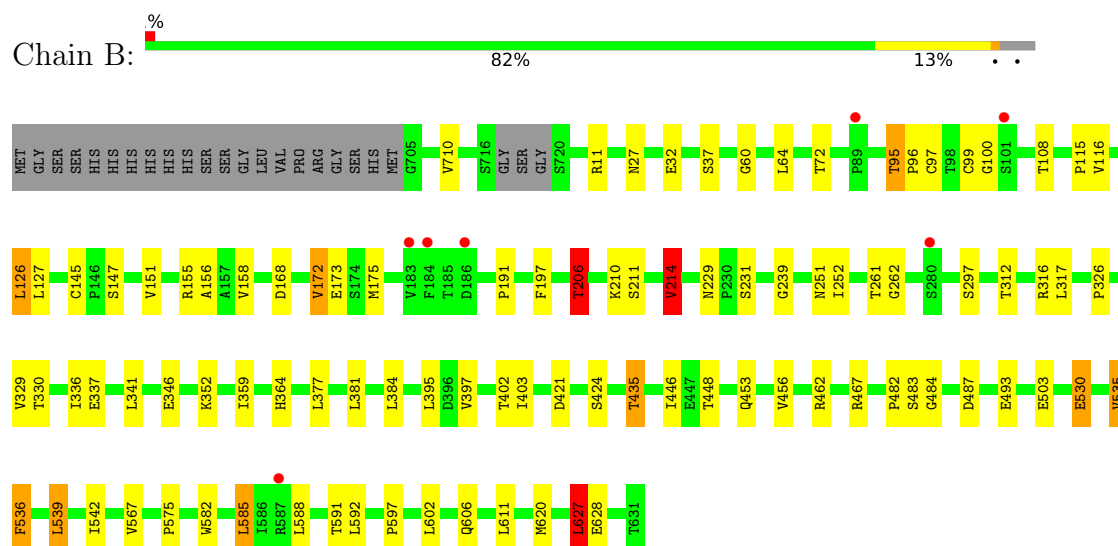
3 Residue-property plots [i](#)

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: HEPATITIS C VIRUS FULL-LENGTH NS3 COMPLEX



• Molecule 1: HEPATITIS C VIRUS FULL-LENGTH NS3 COMPLEX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.37Å 110.50Å 142.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.37 – 2.68 87.37 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.7 (87.37-2.68) 99.2 (87.37-2.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.162 , 0.251 0.162 , 0.245	Depositor DCC
R_{free} test set	2069 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10116	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: UP8

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	1.08	5/4807 (0.1%)	1.36	29/6578 (0.4%)
1	B	1.05	5/4800 (0.1%)	1.32	15/6573 (0.2%)
All	All	1.06	10/9607 (0.1%)	1.34	44/13151 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	LYS	CA-C	6.54	1.59	1.52
1	B	214	VAL	CA-C	5.46	1.58	1.52
1	B	206	THR	CA-C	5.40	1.60	1.52
1	A	620	MET	SD-CE	-5.29	1.66	1.79
1	B	175	MET	SD-CE	-5.29	1.66	1.79
1	A	434	GLN	CA-C	-5.24	1.46	1.52
1	B	620	MET	SD-CE	-5.19	1.66	1.79
1	B	424	SER	C-N	5.17	1.40	1.33
1	A	336	ILE	CA-C	5.15	1.59	1.52
1	A	525	CYS	CA-C	-5.08	1.46	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	VAL	N-CA-CB	8.35	121.25	110.57
1	A	498	GLY	CA-C-N	6.49	129.26	120.44
1	A	498	GLY	C-N-CA	6.49	129.26	120.44
1	B	602	LEU	CA-C-N	6.47	128.40	120.51
1	B	602	LEU	C-N-CA	6.47	128.40	120.51
1	B	206	THR	CB-CA-C	6.03	118.44	110.06
1	A	214	VAL	N-CA-CB	5.92	119.49	111.21
1	A	272	LYS	CA-C-N	5.86	128.05	120.44
1	A	272	LYS	C-N-CA	5.86	128.05	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	PRO	CA-C-N	5.67	127.81	120.44
1	A	194	PRO	C-N-CA	5.67	127.81	120.44
1	A	396	ASP	CA-C-N	5.63	129.37	120.47
1	A	396	ASP	C-N-CA	5.63	129.37	120.47
1	A	481	ARG	CB-CA-C	5.62	117.54	109.11
1	B	214	VAL	N-CA-CB	5.61	119.06	111.21
1	A	527	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	408	VAL	N-CA-CB	5.50	116.72	110.72
1	B	27	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	95	THR	CB-CA-C	5.46	117.29	109.26
1	A	243	SER	CA-C-N	5.41	127.79	120.44
1	A	243	SER	C-N-CA	5.41	127.79	120.44
1	B	536	PHE	CA-C-N	5.38	127.76	120.38
1	B	536	PHE	C-N-CA	5.38	127.76	120.38
1	A	528	HIS	CA-C-N	5.35	127.39	120.44
1	A	528	HIS	C-N-CA	5.35	127.39	120.44
1	A	446	ILE	N-CA-CB	5.33	117.08	111.00
1	B	627	LEU	CA-C-N	-5.32	115.12	122.30
1	B	627	LEU	C-N-CA	-5.32	115.12	122.30
1	A	706	SER	CA-C-N	5.32	129.23	122.37
1	A	706	SER	C-N-CA	5.32	129.23	122.37
1	B	530	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	626	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	460	GLN	CA-C-N	5.26	127.28	120.44
1	A	460	GLN	C-N-CA	5.26	127.28	120.44
1	B	582	TRP	CA-C-N	5.24	127.56	120.38
1	B	582	TRP	C-N-CA	5.24	127.56	120.38
1	A	508	GLU	CA-C-N	5.21	127.69	120.29
1	A	508	GLU	C-N-CA	5.21	127.69	120.29
1	B	446	ILE	N-CA-CB	5.16	117.87	111.41
1	A	507	ALA	CA-C-N	5.15	127.44	120.38
1	A	507	ALA	C-N-CA	5.15	127.44	120.38
1	A	304	GLY	CA-C-N	5.06	127.02	120.44
1	A	304	GLY	C-N-CA	5.06	127.02	120.44
1	A	335	ASN	CA-CB-CG	5.01	117.61	112.60

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	4701	0	4563	46	0
1	B	4692	0	4545	32	0
2	A	13	5	5	1	0
2	B	13	5	5	0	0
3	A	347	0	0	2	0
3	B	340	0	0	1	0
All	All	10106	10	9118	78	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 (78) 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:A:132:VAL:HG11	1:A:159:CYS:SG	2.00	1.00
1:A:596:THR:HG22	1:A:607:ASN:HD22	1.38	0.87
1:B:97:CYS:HG	1:B:145:CYS:HG	1.24	0.84
1:B:229:ASN:HD22	1:B:231:SER:H	1.34	0.75
1:A:596:THR:HG22	1:A:607:ASN:ND2	2.01	0.74
1:A:251:ASN:HD22	1:A:261:THR:H	1.34	0.74
1:A:132:VAL:CG1	1:A:159:CYS:SG	2.76	0.72
1:B:96:PRO:HB3	1:B:172:VAL:HG11	1.74	0.70
1:B:251:ASN:HD22	1:B:261:THR:H	1.42	0.68
1:A:82:LEU:HG	1:A:170:VAL:HG11	1.75	0.67
1:A:210:LYS:HA	1:A:214:VAL:HG13	1.77	0.66
1:B:336:ILE:HD13	1:B:462:ARG:HG2	1.78	0.65
1:A:132:VAL:HG11	1:A:159:CYS:HG	1.61	0.64
1:A:242:MET:HE1	1:A:265:VAL:HG21	1.80	0.64
1:B:326:PRO:HB3	1:B:484:GLY:HA3	1.80	0.63
1:A:337:GLU:HB2	1:A:470:ARG:HH21	1.63	0.63
1:A:294:SER:HB2	1:A:299:THR:HG21	1.83	0.60
1:B:239:GLY:HA3	1:B:252:ILE:HD11	1.84	0.60
1:A:455:ALA:HB3	1:A:483:SER:HB3	1.85	0.58
1:A:229:ASN:HD22	1:A:231:SER:H	1.51	0.58
1:B:156:ALA:HB3	1:B:168:ASP:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASN:ND2	1:B:261:THR:H	2.02	0.57
1:A:132:VAL:HG12	1:A:164:ALA:HB2	1.86	0.55
1:B:210:LYS:HA	1:B:214:VAL:HG13	1.89	0.54
1:A:574:PRO:O	1:A:596:THR:HB	2.07	0.54
1:A:616:THR:HG22	1:A:620:MET:HE2	1.91	0.53
1:B:251:ASN:HD21	1:B:262:GLY:H	1.57	0.53
1:A:251:ASN:ND2	1:A:261:THR:H	2.05	0.52
1:A:8:GLN:HG2	3:A:2010:HOH:O	2.10	0.51
1:A:486:PHE:CE2	1:A:525:CYS:HB2	2.47	0.50
1:A:194:PRO:HG3	1:A:198:GLN:HB2	1.93	0.50
1:B:116:VAL:HG22	1:B:126:LEU:HD12	1.92	0.50
1:A:158:VAL:HB	1:A:166:ALA:HB3	1.93	0.49
1:B:251:ASN:HD21	1:B:262:GLY:N	2.10	0.49
1:A:415:MET:HA	1:A:464:ARG:NH2	2.26	0.49
1:B:421:ASP:HB3	1:B:467:ARG:HD2	1.92	0.49
1:B:575:PRO:HB3	1:B:585:LEU:HD23	1.94	0.49
1:A:391:TYR:O	1:A:410:ALA:HA	2.12	0.49
1:B:297:SER:HB3	1:B:493:GLU:HB3	1.93	0.49
1:B:115:PRO:HB2	1:B:127:LEU:HD22	1.93	0.49
1:B:536:PHE:HA	1:B:539:LEU:HD22	1.95	0.49
1:A:104:LEU:HD11	1:A:151:VAL:HG21	1.96	0.47
1:B:456:VAL:HG23	1:B:483:SER:HB2	1.95	0.47
1:A:293:HIS:CD2	1:A:322:THR:OG1	2.69	0.47
1:B:710:VAL:HA	1:B:11:ARG:HB2	1.97	0.47
1:A:456:VAL:HG23	1:A:483:SER:HB2	1.98	0.46
1:A:410:ALA:HB1	1:A:414:LEU:HB2	1.98	0.45
1:A:482:PRO:HG2	1:A:485:MET:HE1	1.98	0.45
1:A:625:ALA:HB2	3:A:2289:HOH:O	2.15	0.45
1:A:617:LYS:HA	1:A:620:MET:HE3	1.98	0.44
1:B:627:LEU:HD12	1:B:627:LEU:HA	1.87	0.44
1:B:435:THR:HA	1:B:487:ASP:OD2	2.18	0.44
1:A:214:VAL:HG22	1:A:215:PRO:HD3	1.99	0.43
1:A:598:LEU:HD22	1:A:609:VAL:HG11	2.01	0.43
1:A:493:GLU:HG3	1:A:557:PHE:CE1	2.54	0.43
1:B:158:VAL:HG22	1:B:628:GLU:HG3	2.00	0.43
1:A:194:PRO:HD2	1:A:317:LEU:HB2	2.02	0.42
1:A:545:HIS:O	1:A:549:GLN:HG3	2.19	0.42
1:A:210:LYS:HA	1:A:214:VAL:CG1	2.47	0.42
1:B:60:GLY:HA2	1:B:482:PRO:HB3	2.01	0.42
1:B:359:ILE:HA	1:B:364:HIS:CD2	2.55	0.42
1:B:346:GLU:H	1:B:346:GLU:CD	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:O	1:B:381:LEU:HG	2.20	0.41
1:A:335:ASN:HB3	1:A:469:ARG:O	2.19	0.41
1:B:96:PRO:HB3	1:B:172:VAL:CG1	2.47	0.41
1:A:333:HIS:CD2	1:A:335:ASN:H	2.38	0.41
1:B:191:PRO:HG2	1:B:317:LEU:HD21	2.03	0.41
1:A:299:THR:O	1:A:303:ILE:HG13	2.20	0.41
1:A:364:HIS:HB2	1:A:407:VAL:HG22	2.02	0.41
1:A:97:CYS:HA	1:A:149:HIS:CB	2.50	0.41
1:B:206:THR:HG21	3:B:2112:HOH:O	2.19	0.41
1:A:126:LEU:HD13	1:A:167:VAL:HG13	2.02	0.41
1:A:243:SER:HA	1:A:248:ILE:O	2.22	0.40
1:A:301:LEU:HD11	1:A:509:THR:HG23	2.03	0.40
1:B:197:PHE:HA	1:B:316:ARG:O	2.21	0.40
1:B:567:VAL:HG12	1:B:597:PRO:HG2	2.04	0.40
1:A:209:GLY:HA2	2:A:1721:UP8:O8	2.21	0.40
1:A:615:ILE:O	1:A:619:ILE:HG13	2.22	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	638/666 (96%)	612 (96%)	22 (3%)	4 (1%)	21	41
1	B	638/666 (96%)	609 (96%)	27 (4%)	2 (0%)	36	57
All	All	1276/1332 (96%)	1221 (96%)	49 (4%)	6 (0%)	24	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ASP
1	A	100	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	GLY
1	A	403	ILE
1	B	99	CYS
1	B	100	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/544 (92%)	463 (93%)	37 (7%)	13	28
1	B	488/544 (90%)	447 (92%)	41 (8%)	10	23
All	All	988/1088 (91%)	910 (92%)	78 (8%)	11	25

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	64	LEU
1	A	82	LEU
1	A	83	VAL
1	A	86	GLN
1	A	104	LEU
1	A	109	ARG
1	A	114	ILE
1	A	118	ARG
1	A	119	ARG
1	A	126	LEU
1	A	151	VAL
1	A	173	GLU
1	A	195	GLN
1	A	198	GLN
1	A	206	THR
1	A	211	SER
1	A	214	VAL
1	A	224	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	225	VAL
1	A	242	MET
1	A	249	ASP
1	A	301	LEU
1	A	352	LYS
1	A	386	ILE
1	A	397	VAL
1	A	408	VAL
1	A	449	THR
1	A	477	THR
1	A	480	GLU
1	A	529	LEU
1	A	585	LEU
1	A	596	THR
1	A	609	VAL
1	A	611	LEU
1	A	615	ILE
1	A	627	LEU
1	B	32	GLU
1	B	37	SER
1	B	64	LEU
1	B	72	THR
1	B	95	THR
1	B	108	THR
1	B	126	LEU
1	B	147	SER
1	B	151	VAL
1	B	155	ARG
1	B	172	VAL
1	B	173	GLU
1	B	206	THR
1	B	211	SER
1	B	214	VAL
1	B	312	THR
1	B	329	VAL
1	B	330	THR
1	B	337	GLU
1	B	341	LEU
1	B	352	LYS
1	B	384	LEU
1	B	395	LEU
1	B	397	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	402	THR
1	B	403	ILE
1	B	435	THR
1	B	448	THR
1	B	453	GLN
1	B	503	GLU
1	B	530	GLU
1	B	535	VAL
1	B	539	LEU
1	B	542	ILE
1	B	585	LEU
1	B	588	LEU
1	B	591	THR
1	B	592	LEU
1	B	606	GLN
1	B	611	LEU
1	B	627	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	41	GLN
1	A	49	ASN
1	A	198	GLN
1	A	229	ASN
1	A	251	ASN
1	A	293	HIS
1	A	333	HIS
1	A	335	ASN
1	A	460	GLN
1	A	549	GLN
1	A	606	GLN
1	B	77	ASN
1	B	229	ASN
1	B	251	ASN
1	B	343	ASN
1	B	606	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	UP8	B	1721	-	13,13,13	0.85	0	17,18,18	0.87	1 (5%)
2	UP8	A	1721	-	13,13,13	0.89	0	17,18,18	0.88	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UP8	B	1721	-	-	4/8/8/8	0/1/1/1
2	UP8	A	1721	-	-	4/8/8/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	UP8	O8-C7-C6	-2.20	116.72	121.97
2	B	1721	UP8	O8-C7-C6	-2.02	117.14	121.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1721	UP8	C5-C6-C7-O9
2	A	1721	UP8	C5-C6-C7-O8
2	B	1721	UP8	C2-C10-C11-O12
2	A	1721	UP8	C10-C6-C7-O8
2	A	1721	UP8	C10-C6-C7-O9
2	B	1721	UP8	C5-C6-C7-O8
2	B	1721	UP8	C2-C10-C11-O13
2	B	1721	UP8	C5-C6-C7-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	UP8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	643/666 (96%)	-0.27	10 (1%) 70 68	11, 35, 68, 87	0
1	B	642/666 (96%)	-0.26	7 (1%) 78 76	15, 36, 61, 81	0
All	All	1285/1332 (96%)	-0.27	17 (1%) 75 73	11, 36, 64, 87	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ILE	3.0
1	A	98	THR	2.8
1	B	101	SER	2.8
1	A	246	HIS	2.8
1	B	184	PHE	2.8
1	B	89	PRO	2.7
1	A	182	PRO	2.7
1	A	185	THR	2.5
1	B	587	ARG	2.5
1	B	186	ASP	2.3
1	A	90	GLY	2.2
1	A	247	GLY	2.2
1	A	280	SER	2.2
1	A	357	GLU	2.1
1	A	207	GLY	2.1
1	B	183	VAL	2.1
1	B	280	SER	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	UP8	B	1721	13/13	0.79	0.12	58,73,74,75	0
2	UP8	A	1721	13/13	0.88	0.09	35,41,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.