



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:46 PM UTC

PDB ID : 6H80 / pdb_00006h80
Title : Dengue-RdRp3-inhibitor complex co-crystallisation
Authors : Talapatra, S.K.; Kozielski, F.
Deposited on : 2018-07-31
Resolution : 2.30 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

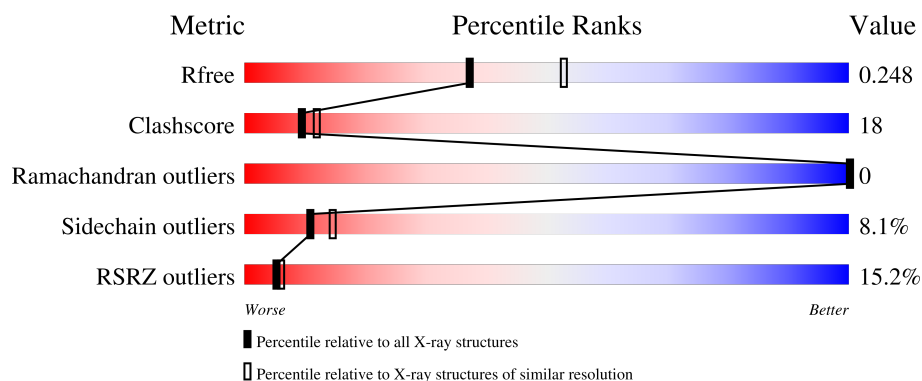
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	635	

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
3	ZN	A	1003	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4747 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.

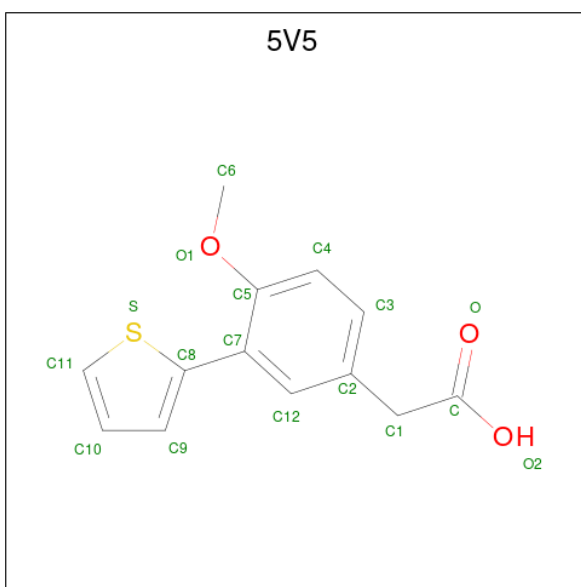
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	558	4529	2865	814	819	31	0	3	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	-	expression tag	UNP Q6YMS4
A	267	SER	-	expression tag	UNP Q6YMS4
A	268	HIS	-	expression tag	UNP Q6YMS4
A	269	MET	-	expression tag	UNP Q6YMS4
A	270	LEU	-	expression tag	UNP Q6YMS4
A	271	ASP	-	expression tag	UNP Q6YMS4
A	366	LEU	MET	variant	UNP Q6YMS4
A	372	VAL	ALA	variant	UNP Q6YMS4
A	480	VAL	ALA	variant	UNP Q6YMS4
A	603	VAL	LEU	variant	UNP Q6YMS4

- Molecule 2 is 2-(4-methoxy-3-thiophen-2-yl-phenyl)ethanoic acid (CCD ID: 5V5) (formula: C₁₃H₁₂O₃S).

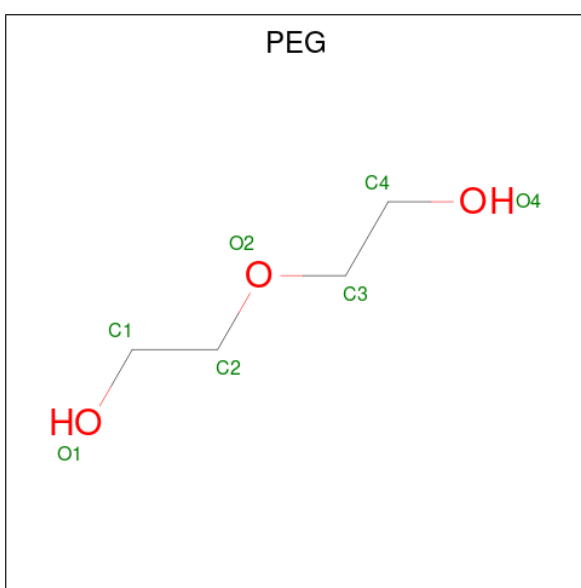


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			17	13	3	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	164	Total	O	0	0
			164	164		

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: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.08Å 181.25Å 57.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 2.30 52.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.70-2.30) 99.9 (52.70-2.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.191 , 0.236 0.231 , 0.248	Depositor DCC
R_{free} test set	1946 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.9	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	0.94	EDS
Total number of atoms	4747	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5V5, PEG

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	1.69	62/4642 (1.3%)	1.48	36/6293 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	HIS	CE1-NE2	-12.92	1.19	1.32
1	A	441	HIS	CE1-NE2	-9.80	1.22	1.32
1	A	714	HIS	CE1-NE2	-9.15	1.23	1.32
1	A	669	PRO	C-O	-7.97	1.13	1.23
1	A	365	PRO	C-O	-7.88	1.14	1.23
1	A	727	PRO	C-O	-7.28	1.14	1.24
1	A	390	PRO	C-O	-7.17	1.15	1.23
1	A	730	PRO	C-O	-7.02	1.15	1.23
1	A	712	HIS	CA-CB	7.00	1.63	1.53
1	A	692	PRO	C-O	-6.96	1.15	1.23
1	A	671	ASP	C-O	-6.96	1.17	1.24
1	A	525	PRO	C-O	-6.67	1.16	1.23
1	A	441	HIS	CA-CB	6.63	1.64	1.53
1	A	707	PRO	C-O	-6.62	1.15	1.24
1	A	696	PRO	C-O	-6.60	1.15	1.23
1	A	822	PRO	C-O	-6.55	1.15	1.24
1	A	837	PRO	C-O	-6.54	1.15	1.23
1	A	367	PRO	C-O	-6.41	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	636	PRO	C-O	-6.37	1.16	1.24
1	A	385	GLY	C-O	-6.32	1.18	1.24
1	A	558	PRO	C-O	-6.20	1.16	1.24
1	A	829	PRO	C-O	-6.16	1.16	1.23
1	A	437	GLU	CD-OE2	-6.02	1.14	1.25
1	A	789	PRO	C-O	-5.99	1.17	1.23
1	A	532	ASP	C-O	-5.95	1.16	1.24
1	A	654	ARG	C-O	-5.93	1.17	1.24
1	A	363	PRO	C-O	-5.85	1.17	1.23
1	A	330	PRO	C-O	-5.82	1.16	1.24
1	A	735	ILE	C-O	-5.79	1.17	1.24
1	A	608	LEU	C-O	-5.71	1.17	1.24
1	A	711	HIS	C-O	-5.64	1.17	1.23
1	A	611	PHE	C-O	-5.63	1.17	1.24
1	A	646	TRP	C-O	-5.62	1.17	1.24
1	A	541	ILE	C-O	-5.59	1.18	1.24
1	A	667	VAL	C-O	-5.59	1.18	1.24
1	A	437	GLU	N-CA	5.51	1.53	1.46
1	A	519	ARG	C-O	-5.51	1.17	1.24
1	A	711	HIS	CE1-NE2	-5.49	1.27	1.32
1	A	335	PRO	C-O	-5.47	1.17	1.24
1	A	684	MET	C-O	-5.44	1.16	1.24
1	A	725	VAL	C-O	-5.44	1.18	1.24
1	A	715	GLU	C-O	-5.42	1.17	1.24
1	A	545	ASP	C-O	-5.41	1.17	1.24
1	A	714	HIS	CA-CB	5.39	1.61	1.53
1	A	550	GLU	C-O	-5.38	1.17	1.24
1	A	617	GLN	C-O	-5.35	1.17	1.24
1	A	666	VAL	C-O	-5.21	1.18	1.24
1	A	717	ILE	C-O	-5.19	1.18	1.24
1	A	658	MET	C-O	-5.15	1.17	1.23
1	A	548	ASN	C-O	-5.15	1.18	1.24
1	A	368	GLY	C-O	-5.14	1.17	1.23
1	A	731	GLN	C-O	-5.12	1.17	1.24
1	A	643	ILE	C-O	-5.10	1.18	1.24
1	A	657	ARG	C-O	-5.09	1.17	1.24
1	A	610	THR	C-O	-5.05	1.18	1.24
1	A	298	PRO	C-O	-5.04	1.17	1.24
1	A	767	PHE	C-O	-5.04	1.17	1.24
1	A	784	PRO	C-O	-5.01	1.18	1.23
1	A	859	TRP	C-O	-5.01	1.18	1.24
1	A	621	GLN	C-O	-5.00	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	668	LYS	C-O	-5.00	1.18	1.24
1	A	702	ASP	C-O	-5.00	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	712	HIS	CA-CB-CG	16.16	129.96	113.80
1	A	714	HIS	CA-CB-CG	15.44	129.24	113.80
1	A	441	HIS	CA-CB-CG	14.51	128.31	113.80
1	A	437	GLU	CB-CG-CD	13.57	135.68	112.60
1	A	714	HIS	CB-CA-C	10.85	127.44	109.53
1	A	441	HIS	CB-CA-C	10.23	129.55	110.63
1	A	436	ARG	CA-C-O	-9.53	111.09	120.90
1	A	449	CYS	CB-CA-C	9.29	126.70	111.83
1	A	712	HIS	ND1-CG-CD2	-8.93	97.17	106.10
1	A	441	HIS	ND1-CG-CD2	-8.33	97.77	106.10
1	A	712	HIS	CB-CA-C	8.02	122.76	109.53
1	A	714	HIS	ND1-CG-CD2	-7.83	98.27	106.10
1	A	437	GLU	N-CA-CB	7.78	122.20	110.22
1	A	711	HIS	CA-C-N	7.68	133.46	122.09
1	A	711	HIS	C-N-CA	7.68	133.46	122.09
1	A	877	GLU	CA-C-N	-7.52	112.34	122.72
1	A	877	GLU	C-N-CA	-7.52	112.34	122.72
1	A	437	GLU	N-CA-C	-7.35	103.26	111.71
1	A	728	CYS	CB-CA-C	7.24	121.64	109.48
1	A	728	CYS	N-CA-CB	7.19	122.39	110.52
1	A	728	CYS	CA-CB-SG	7.08	130.68	114.40
1	A	452	ASN	CB-CA-C	-6.94	96.56	110.30
1	A	741	SER	CA-C-N	-6.88	113.62	122.77
1	A	741	SER	C-N-CA	-6.88	113.62	122.77
1	A	729	ARG	CB-CA-C	6.36	119.83	109.97
1	A	445	LYS	CA-C-O	-5.71	115.16	121.33
1	A	510	GLY	CA-C-O	-5.69	118.31	122.23
1	A	714	HIS	CG-CD2-NE2	5.60	112.80	107.20
1	A	436	ARG	N-CA-C	5.50	117.13	111.03
1	A	272	ASN	CA-C-N	5.37	128.01	120.28
1	A	272	ASN	C-N-CA	5.37	128.01	120.28
1	A	290	THR	CA-C-N	-5.33	115.91	122.84
1	A	290	THR	C-N-CA	-5.33	115.91	122.84
1	A	727	PRO	N-CA-CB	-5.26	97.72	103.25
1	A	441	HIS	N-CA-C	-5.15	105.78	111.71
1	A	435	ASP	N-CA-C	-5.04	105.92	111.71

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	389	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	403	ARG	Sidechain
1	A	419	ASP	Peptide
1	A	436	ARG	Sidechain
1	A	471	ARG	Sidechain
1	A	547[A]	HIS	Mainchain
1	A	561	ARG	Sidechain
1	A	594	ARG	Sidechain
1	A	739	ARG	Sidechain
1	A	773	ARG	Sidechain
1	A	785	VAL	Mainchain
1	A	786[A]	HIS	Mainchain
1	A	792	ARG	Sidechain
1	A	815	ARG	Sidechain
1	A	842	ARG	Sidechain

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	4529	0	4355	160	1
2	A	17	0	0	0	0
3	A	2	0	0	2	0
4	A	35	0	50	2	0
5	A	164	0	0	14	0
All	All	4747	0	4405	161	1

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 18.

All (161) 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:712:HIS:HD2	1:A:714:HIS:NE2	1.25	1.30
1:A:764[A]:LEU:HD23	1:A:809:MET:CE	1.64	1.27
1:A:712:HIS:CD2	3:A:1003:ZN:ZN	1.22	1.23
1:A:712:HIS:NE2	1:A:728:CYS:HB3	1.54	1.21
1:A:712:HIS:CD2	1:A:714:HIS:NE2	2.08	1.20
1:A:437:GLU:OE1	1:A:447:GLY:N	1.78	1.16
1:A:437:GLU:OE2	1:A:448:SER:OG	1.64	1.14
1:A:712:HIS:CD2	1:A:728:CYS:HB2	1.82	1.11
1:A:712:HIS:CE1	1:A:728:CYS:HB3	1.85	1.10
1:A:371:LYS:NZ	1:A:638:LEU:O	1.83	1.10
1:A:728:CYS:SG	1:A:839:LEU:HD11	1.91	1.09
1:A:484:GLU:OE1	1:A:572:TYR:OH	1.70	1.08
1:A:764[A]:LEU:CD2	1:A:809:MET:HE3	1.82	1.07
1:A:712:HIS:NE2	1:A:728:CYS:CB	2.18	1.06
1:A:448:SER:HB3	1:A:476:MET:HE2	1.33	1.06
1:A:863:ILE:HG21	1:A:883:MET:CE	1.85	1.05
1:A:307:SER:HB2	1:A:589:MET:O	1.54	1.04
1:A:764[A]:LEU:CD2	1:A:809:MET:CE	2.36	1.03
1:A:441:HIS:NE2	1:A:567:ILE:HD13	1.75	1.02
1:A:746:TRP:HE3	1:A:750:GLU:OE1	1.43	1.01
1:A:441:HIS:CE1	1:A:566:ALA:C	2.39	1.00
1:A:712:HIS:HD2	1:A:714:HIS:CD2	1.83	0.96
1:A:441:HIS:CD2	5:A:1151:HOH:O	2.19	0.95
1:A:437:GLU:CD	1:A:448:SER:HG	1.76	0.94
1:A:712:HIS:CD2	1:A:714:HIS:CD2	2.55	0.93
1:A:507:GLU:OE1	5:A:1103:HOH:O	1.87	0.91
1:A:764[A]:LEU:HD23	1:A:809:MET:HE2	1.50	0.91
1:A:712:HIS:CD2	1:A:728:CYS:CB	2.51	0.90
1:A:301:THR:HB	1:A:359:ASP:OD1	1.73	0.88
1:A:712:HIS:NE2	3:A:1003:ZN:ZN	1.37	0.87
1:A:863:ILE:HG21	1:A:883:MET:HE1	1.56	0.86
1:A:437:GLU:CD	1:A:448:SER:H	1.83	0.85
1:A:578:LYS:HB3	1:A:589:MET:HE2	1.58	0.84
1:A:764[A]:LEU:HD21	1:A:809:MET:HE3	1.59	0.84
1:A:863:ILE:CG2	1:A:883:MET:CE	2.55	0.84
1:A:448:SER:CB	1:A:476:MET:HE2	2.08	0.84
1:A:863:ILE:CG2	1:A:883:MET:HE2	2.09	0.83
1:A:746:TRP:CE3	1:A:750:GLU:OE1	2.33	0.82
1:A:441:HIS:NE2	1:A:567:ILE:CD1	2.43	0.81
1:A:441:HIS:HE1	1:A:566:ALA:C	1.89	0.80
1:A:437:GLU:OE1	1:A:448:SER:N	2.14	0.79
1:A:746:TRP:CE3	1:A:750:GLU:CD	2.61	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLU:CD	1:A:448:SER:N	2.42	0.78
1:A:712:HIS:CE1	1:A:728:CYS:CB	2.60	0.78
1:A:712:HIS:NE2	1:A:847:CYS:SG	2.57	0.77
1:A:441:HIS:CE1	1:A:567:ILE:N	2.53	0.77
1:A:307:SER:CB	1:A:589:MET:O	2.33	0.76
1:A:437:GLU:OE1	1:A:447:GLY:CA	2.32	0.76
1:A:712:HIS:ND1	1:A:728:CYS:C	2.46	0.74
1:A:728:CYS:SG	1:A:839:LEU:CD1	2.76	0.72
1:A:401:LYS:HE3	1:A:493:GLU:OE2	1.88	0.72
1:A:746:TRP:HE3	1:A:750:GLU:CD	1.97	0.72
1:A:712:HIS:CE1	1:A:728:CYS:C	2.68	0.71
1:A:302:TRP:CE3	1:A:592:ILE:HG13	2.25	0.71
1:A:712:HIS:CE1	1:A:729:ARG:N	2.58	0.70
1:A:437:GLU:CD	1:A:448:SER:OG	2.28	0.70
1:A:389:ARG:HH12	1:A:557:ASP:CG	1.98	0.70
1:A:403:ARG:HH21	1:A:426:GLU:CD	2.00	0.70
1:A:302:TRP:CZ3	1:A:594:ARG:HG2	2.27	0.69
1:A:441:HIS:HE1	1:A:566:ALA:O	1.76	0.69
1:A:441:HIS:HD2	5:A:1151:HOH:O	1.62	0.69
1:A:441:HIS:CE1	1:A:567:ILE:HA	2.27	0.69
1:A:770:ARG:HD3	1:A:851:ILE:HD13	1.74	0.69
1:A:395:ARG:HD2	1:A:431:TRP:CD2	2.28	0.68
1:A:429:GLU:OE1	1:A:429:GLU:N	2.27	0.68
1:A:437:GLU:OE2	1:A:448:SER:CB	2.42	0.67
1:A:441:HIS:CE1	1:A:566:ALA:O	2.48	0.67
1:A:448:SER:HB3	1:A:476:MET:CE	2.18	0.66
1:A:471:ARG:N	1:A:471:ARG:HD2	2.10	0.66
1:A:296:GLU:HG2	1:A:296:GLU:O	1.95	0.65
1:A:422:LYS:O	1:A:426:GLU:HG2	1.97	0.65
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.79	0.65
1:A:302:TRP:CE2	1:A:594:ARG:HD2	2.32	0.64
1:A:437:GLU:OE2	1:A:448:SER:N	2.31	0.64
1:A:301:THR:CB	1:A:359:ASP:OD1	2.44	0.64
1:A:798:HIS:HD2	5:A:1155:HOH:O	1.80	0.64
1:A:441:HIS:ND1	1:A:566:ALA:HB1	2.14	0.63
1:A:441:HIS:HD1	1:A:570:LEU:HD12	1.63	0.62
1:A:495:HIS:ND1	5:A:1103:HOH:O	1.81	0.60
1:A:792:ARG:HD3	1:A:795:TRP:CE2	2.36	0.60
1:A:441:HIS:CE1	1:A:567:ILE:HD13	2.34	0.60
1:A:441:HIS:CE1	1:A:567:ILE:CA	2.84	0.59
1:A:712:HIS:HD2	1:A:714:HIS:CE1	2.09	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:TYR:CE1	1:A:304:TYR:CD2	2.91	0.59
1:A:293:TYR:CE1	1:A:304:TYR:HD2	2.20	0.59
1:A:420:SER:O	1:A:420:SER:OG	2.09	0.59
1:A:441:HIS:HE1	1:A:567:ILE:HA	1.68	0.58
1:A:764[A]:LEU:HD23	1:A:809:MET:HE3	1.44	0.58
1:A:395:ARG:HD2	1:A:431:TRP:CE2	2.37	0.58
1:A:712:HIS:CD2	1:A:847:CYS:SG	2.97	0.58
1:A:437:GLU:O	1:A:441:HIS:N	2.22	0.58
1:A:547[A]:HIS:CE1	5:A:1124:HOH:O	2.57	0.57
1:A:401:LYS:CE	1:A:493:GLU:OE2	2.51	0.57
1:A:559:GLU:H	1:A:559:GLU:CD	2.12	0.57
1:A:879:PHE:HA	5:A:1112:HOH:O	2.03	0.57
1:A:871:ARG:HG2	1:A:879:PHE:CE2	2.40	0.57
1:A:712:HIS:HE2	1:A:728:CYS:HB3	1.61	0.56
1:A:279:ARG:HB2	5:A:1136:HOH:O	2.06	0.55
1:A:389:ARG:NH1	1:A:557:ASP:OD2	2.39	0.55
1:A:680:ALA:O	1:A:684:MET:HG3	2.07	0.55
1:A:403:ARG:NH2	1:A:426:GLU:OE2	2.31	0.55
1:A:747:SER:OG	1:A:750:GLU:HG3	2.07	0.55
1:A:336:MET:CE	1:A:340:MET:HG3	2.37	0.54
1:A:587:THR:C	1:A:588:VAL:CG1	2.79	0.54
1:A:851:ILE:HA	1:A:856:ARG:HD2	1.90	0.54
1:A:289:SER:C	1:A:290:THR:CG2	2.81	0.54
1:A:871:ARG:HG2	1:A:879:PHE:CD2	2.43	0.54
1:A:329:LYS:N	1:A:330:PRO:CD	2.71	0.53
1:A:779:ILE:O	1:A:783:VAL:HG13	2.08	0.53
1:A:277:GLY:O	1:A:281:LYS:HG2	2.09	0.52
1:A:863:ILE:N	1:A:864:PRO:CD	2.73	0.52
1:A:290:THR:O	1:A:290:THR:OG1	2.24	0.51
1:A:336:MET:HE2	1:A:340:MET:HG3	1.91	0.51
1:A:441:HIS:HE1	1:A:567:ILE:CA	2.23	0.51
1:A:289:SER:C	1:A:290:THR:HG23	2.37	0.50
1:A:287:HIS:O	1:A:291:TRP:HB2	2.12	0.50
1:A:294:ASP:OD1	1:A:296:GLU:HB3	2.12	0.49
1:A:437:GLU:OE1	1:A:447:GLY:C	2.55	0.49
1:A:441:HIS:CE1	1:A:566:ALA:CB	2.95	0.49
1:A:600:SER:OG	1:A:601:GLY:N	2.45	0.49
1:A:292:HIS:N	1:A:292:HIS:ND1	2.59	0.49
1:A:654:ARG:HH12	4:A:1007:PEG:H42	1.79	0.48
1:A:869:GLN:O	1:A:873:LEU:HD12	2.13	0.48
1:A:792:ARG:HD3	1:A:795:TRP:CZ2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TRP:CZ2	1:A:594:ARG:HD2	2.50	0.47
1:A:426:GLU:HA	1:A:426:GLU:OE1	2.14	0.47
1:A:286:GLU:O	1:A:286:GLU:HG3	2.13	0.47
1:A:550:GLU:OE1	1:A:573:GLN:NE2	2.43	0.45
1:A:746:TRP:CZ3	1:A:750:GLU:OE2	2.69	0.45
1:A:705:GLN:NE2	5:A:1113:HOH:O	2.43	0.45
1:A:701:HIS:ND1	5:A:1108:HOH:O	2.35	0.45
1:A:441:HIS:NE2	1:A:567:ILE:CG1	2.80	0.44
1:A:851:ILE:HD12	1:A:856:ARG:CZ	2.48	0.44
1:A:389:ARG:HD2	5:A:1249:HOH:O	2.18	0.44
1:A:388:LYS:HG3	5:A:1128:HOH:O	2.17	0.44
1:A:863:ILE:HG22	1:A:883:MET:HE2	1.97	0.44
1:A:334:VAL:HA	1:A:335:PRO:HD3	1.85	0.43
1:A:728:CYS:SG	1:A:768:HIS:CE1	3.12	0.43
1:A:550:GLU:O	1:A:553:ILE:HB	2.19	0.43
1:A:774:LEU:HD22	1:A:859:TRP:CH2	2.54	0.42
1:A:481:ARG:HD3	1:A:481:ARG:HA	1.87	0.42
1:A:656:LYS:NZ	5:A:1104:HOH:O	2.23	0.42
1:A:448:SER:HB2	1:A:476:MET:HG2	2.01	0.42
1:A:599:GLY:HA3	1:A:602:GLN:CD	2.45	0.41
1:A:441:HIS:CE1	1:A:566:ALA:HB1	2.55	0.41
1:A:537:TRP:CD1	1:A:537:TRP:C	2.98	0.41
1:A:429:GLU:OE1	1:A:429:GLU:CA	2.69	0.41
1:A:594:ARG:HE	1:A:594:ARG:HB2	1.65	0.41
4:A:1007:PEG:H12	5:A:1218:HOH:O	2.20	0.41
1:A:635:ASN:HA	1:A:636:PRO:HD3	1.82	0.41
1:A:728:CYS:SG	1:A:768:HIS:HE1	2.43	0.41
1:A:863:ILE:HD13	1:A:863:ILE:HA	1.96	0.41
1:A:712:HIS:CE1	1:A:728:CYS:CA	3.02	0.41
1:A:289:SER:O	1:A:290:THR:HG22	2.19	0.41
1:A:728:CYS:SG	1:A:769:ARG:HD3	2.61	0.41
1:A:297:ASN:HA	1:A:298:PRO:HD3	1.86	0.40
1:A:440:LEU:C	1:A:445:LYS:O	2.65	0.40
1:A:746:TRP:CZ3	1:A:750:GLU:CD	2.98	0.40
1:A:768:HIS:CD2	1:A:768:HIS:H	2.38	0.40
1:A:575:LYS:O	1:A:593:SER:HA	2.22	0.40
1:A:689:LYS:HE2	1:A:689:LYS:HB2	1.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:CG2	1:A:333:VAL:CG2[3_654]	1.82	0.38

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	549/635 (86%)	535 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	473/552 (86%)	435 (92%)	38 (8%)	11	15

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	A	285	GLU
1	A	292	HIS
1	A	326	LEU
1	A	333	VAL
1	A	361	ARG
1	A	364	ARG
1	A	371	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	402	VAL
1	A	405	ASN
1	A	429	GLU
1	A	442	LYS
1	A	450	VAL
1	A	452	ASN
1	A	453	MET
1	A	470	SER
1	A	471	ARG
1	A	473	ILE
1	A	550	GLU
1	A	553	ILE
1	A	575	LYS
1	A	577	VAL
1	A	588	VAL
1	A	589	MET
1	A	592	ILE
1	A	689	LYS
1	A	742	GLN
1	A	746	TRP
1	A	783	VAL
1	A	790	THR
1	A	791	SER
1	A	792	ARG
1	A	797	ILE
1	A	851	ILE
1	A	855	SER
1	A	863	ILE
1	A	874	ILE
1	A	876	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	562	GLN
1	A	712	HIS
1	A	768	HIS
1	A	862	ASN

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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
4	PEG	A	1005	-	6,6,6	0.47	0	5,5,5	0.68	0
4	PEG	A	1006	-	6,6,6	0.50	0	5,5,5	0.55	0
4	PEG	A	1004	-	6,6,6	0.48	0	5,5,5	0.53	0
4	PEG	A	1007	-	6,6,6	0.60	0	5,5,5	0.34	0
2	5V5	A	1001	-	18,18,18	1.44	2 (11%)	24,24,24	1.62	4 (16%)
4	PEG	A	1008	-	6,6,6	0.69	0	5,5,5	0.80	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	PEG	A	1005	-	-	1/4/4/4	-
4	PEG	A	1006	-	-	3/4/4/4	-
4	PEG	A	1004	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	1007	-	-	2/4/4/4	-
2	5V5	A	1001	-	-	0/10/10/10	0/2/2/2
4	PEG	A	1008	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	5V5	C7-C8	3.53	1.53	1.48
2	A	1001	5V5	O1-C5	3.28	1.42	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	5V5	C11-S-C8	4.03	99.83	92.68
2	A	1001	5V5	C10-C11-S	-3.65	104.10	113.02
2	A	1001	5V5	C2-C1-C	-2.17	107.55	113.71
2	A	1001	5V5	C5-C7-C8	-2.15	120.19	123.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	PEG	O2-C3-C4-O4
4	A	1008	PEG	O2-C3-C4-O4
4	A	1004	PEG	O1-C1-C2-O2
4	A	1006	PEG	O1-C1-C2-O2
4	A	1008	PEG	C1-C2-O2-C3
4	A	1007	PEG	C1-C2-O2-C3
4	A	1008	PEG	C4-C3-O2-C2
4	A	1007	PEG	C4-C3-O2-C2
4	A	1006	PEG	C1-C2-O2-C3
4	A	1004	PEG	C4-C3-O2-C2
4	A	1008	PEG	O1-C1-C2-O2
4	A	1006	PEG	O2-C3-C4-O4
4	A	1005	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1007	PEG	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, 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	558/635 (87%)	0.80	85 (15%) 5 6	26, 57, 101, 122	3 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	HIS	10.5
1	A	592	ILE	6.7
1	A	728	CYS	6.0
1	A	477	TRP	5.4
1	A	296	GLU	5.3
1	A	319	MET	5.3
1	A	601	GLY	5.0
1	A	580	GLN	4.9
1	A	712	HIS	4.7
1	A	310	VAL	4.4
1	A	333	VAL	4.4
1	A	402	VAL	4.3
1	A	289	SER	4.2
1	A	293	TYR	4.1
1	A	579	VAL	4.1
1	A	450	VAL	4.0
1	A	299	TYR	4.0
1	A	342	MET	3.9
1	A	436	ARG	3.9
1	A	547[A]	HIS	3.7
1	A	591	ILE	3.7
1	A	311	LYS	3.6
1	A	473	ILE	3.5
1	A	472	ALA	3.5
1	A	451	TYR	3.5
1	A	295	ASP	3.5
1	A	419	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	588	VAL	3.4
1	A	600	SER	3.4
1	A	449	CYS	3.3
1	A	361	ARG	3.3
1	A	309	GLU	3.2
1	A	420	SER	3.1
1	A	404	THR	3.1
1	A	452	ASN	3.1
1	A	272	ASN	3.1
1	A	274	ASP	3.0
1	A	290	THR	3.0
1	A	421	ALA	3.0
1	A	437	GLU	3.0
1	A	746	TRP	3.0
1	A	603	VAL	3.0
1	A	291	TRP	3.0
1	A	304	TYR	2.9
1	A	405	ASN	2.9
1	A	790	THR	2.8
1	A	298	PRO	2.8
1	A	745	GLY	2.8
1	A	453	MET	2.8
1	A	470	SER	2.7
1	A	576	VAL	2.7
1	A	883	MET	2.7
1	A	433	LEU	2.7
1	A	481	ARG	2.6
1	A	307	SER	2.6
1	A	403	ARG	2.6
1	A	478	LEU	2.5
1	A	303	ALA	2.5
1	A	401	LYS	2.5
1	A	645	GLN	2.5
1	A	744	ALA	2.5
1	A	357	LYS	2.4
1	A	676	ASN	2.4
1	A	447	GLY	2.4
1	A	292	HIS	2.4
1	A	355	LYS	2.4
1	A	808	ASP	2.4
1	A	714	HIS	2.3
1	A	880	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	302	TRP	2.3
1	A	471	ARG	2.3
1	A	474	TRP	2.2
1	A	358	VAL	2.2
1	A	786[A]	HIS	2.2
1	A	587	THR	2.2
1	A	283	ILE	2.2
1	A	476	MET	2.1
1	A	602	GLN	2.1
1	A	599	GLY	2.1
1	A	294	ASP	2.1
1	A	448	SER	2.1
1	A	273	MET	2.1
1	A	398	PHE	2.1
1	A	801	HIS	2.0
1	A	881	ASP	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(Å ²)	Q<0.9
4	PEG	A	1008	7/7	0.75	0.25	64,66,74,76	0
4	PEG	A	1006	7/7	0.77	0.20	60,64,72,75	0
4	PEG	A	1005	7/7	0.80	0.18	66,78,79,80	0
4	PEG	A	1007	7/7	0.82	0.17	75,79,80,85	0
4	PEG	A	1004	7/7	0.84	0.16	63,71,75,78	0
2	5V5	A	1001	17/17	0.93	0.10	43,51,65,69	0
3	ZN	A	1002	1/1	0.94	0.06	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1003	1/1	0.98	0.08	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.