



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:21 PM UTC

PDB ID : 4FOL / pdb_00004fol
Title : S-formylglutathione hydrolase Variant H160I
Authors : Legler, P.M.; Millard, C.B.
Deposited on : 2012-06-20
Resolution : 2.07 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
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

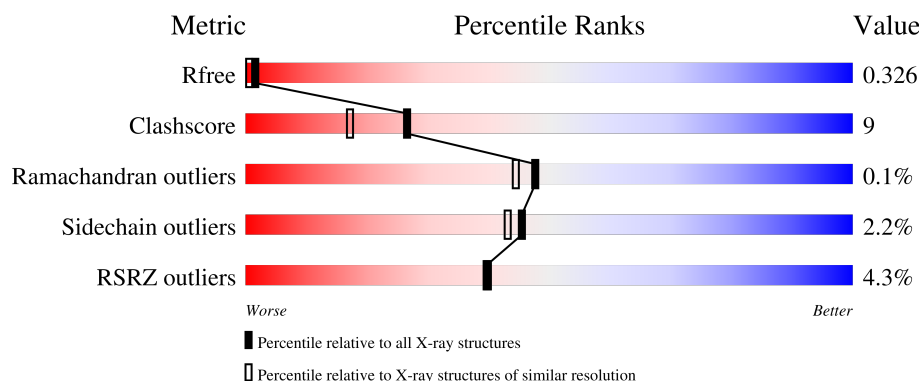
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	299	
1	B	299	
1	C	299	
1	D	299	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9246 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 S-formylglutathione hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2270	1468	375	418	9			
1	B	283	Total	C	N	O	S	0	0	0
			2270	1468	374	419	9			
1	C	282	Total	C	N	O	S	0	0	0
			2261	1462	373	417	9			
1	D	282	Total	C	N	O	S	0	1	0
			2262	1464	370	419	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ILE	HIS	engineered mutation	UNP P40363
B	160	ILE	HIS	engineered mutation	UNP P40363
C	160	ILE	HIS	engineered mutation	UNP P40363
D	160	ILE	HIS	engineered mutation	UNP P40363

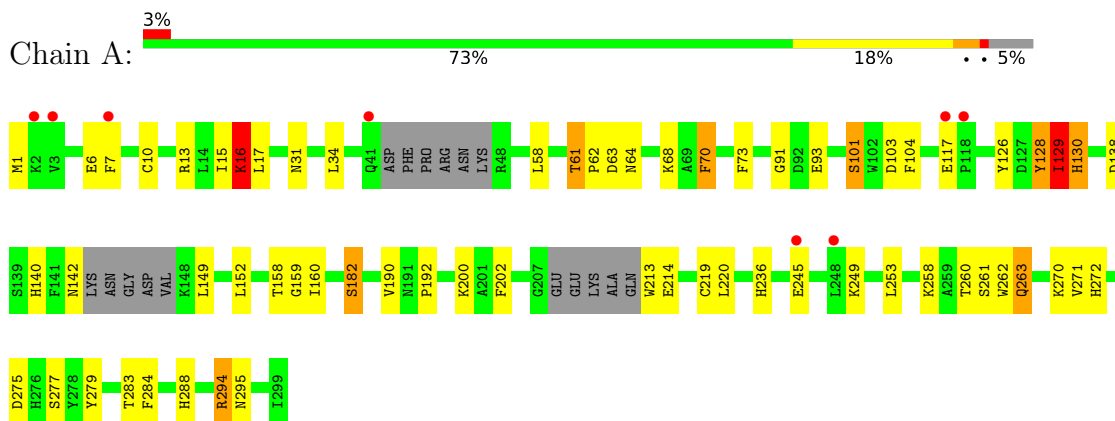
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		
2	B	45	Total	O	0	0
			45	45		
2	C	40	Total	O	0	0
			40	40		
2	D	50	Total	O	0	0
			50	50		

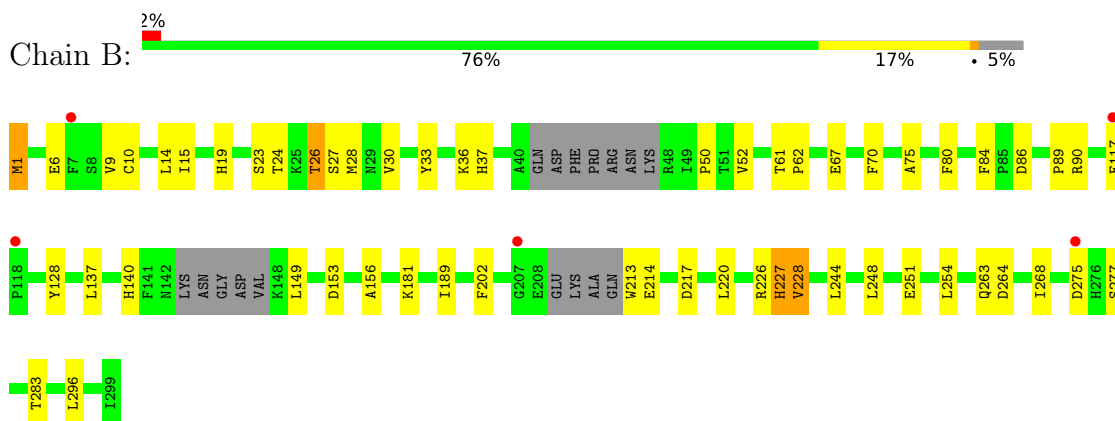
3 Residue-property plots

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.

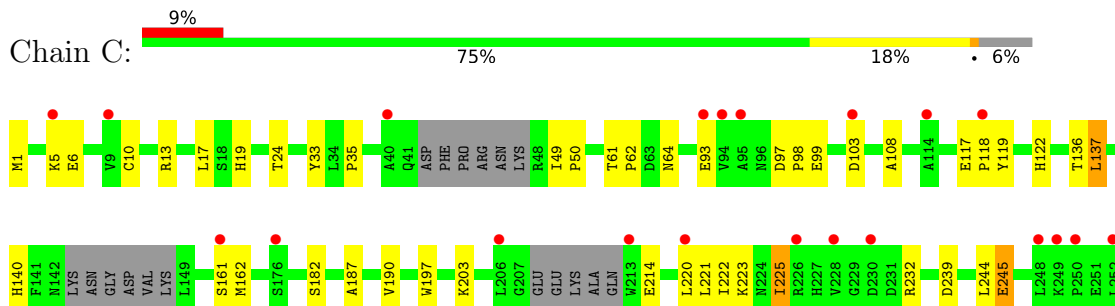
- Molecule 1: S-formylglutathione hydrolase

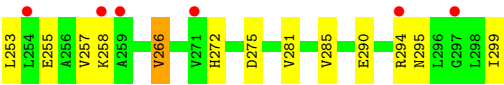


- Molecule 1: S-formylglutathione hydrolase

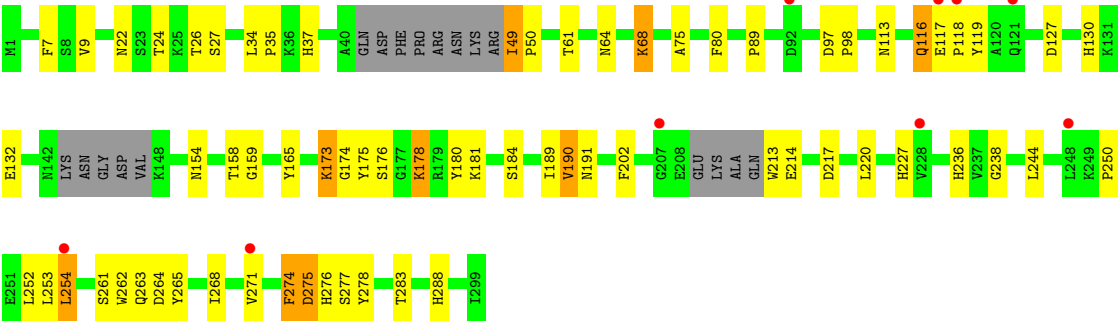


- Molecule 1: S-formylglutathione hydrolase





● Molecule 1: S-formylglutathione hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.30Å 119.74Å 169.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.73 – 2.07 61.73 – 2.07	Depositor EDS
% Data completeness (in resolution range)	90.9 (61.73-2.07) 90.9 (61.73-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.281 , 0.327 0.281 , 0.326	Depositor DCC
R_{free} test set	4145 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.28% 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

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	0.86	6/2339 (0.3%)	0.91	4/3169 (0.1%)
1	B	0.91	7/2339 (0.3%)	0.95	5/3169 (0.2%)
1	C	0.86	3/2330 (0.1%)	0.89	3/3158 (0.1%)
1	D	0.96	9/2334 (0.4%)	1.00	11/3163 (0.3%)
All	All	0.90	25/9342 (0.3%)	0.94	23/12659 (0.2%)

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	D	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	HIS	CG-ND1	-8.68	1.28	1.38
1	B	227	HIS	CD2-NE2	-8.18	1.28	1.37
1	A	126	TYR	C-O	-8.03	1.14	1.24
1	D	262	TRP	NE1-CE2	-7.76	1.28	1.37
1	C	203	LYS	C-O	-6.95	1.16	1.24
1	A	129	ILE	C-O	-6.87	1.16	1.24
1	D	276	HIS	CG-ND1	-6.79	1.30	1.38
1	A	128	TYR	C-O	-6.65	1.16	1.24
1	B	227	HIS	N-CA	-6.53	1.37	1.46
1	B	226	ARG	C-O	-6.43	1.16	1.23
1	D	277	SER	C-O	-6.41	1.15	1.23
1	D	178	LYS	C-O	-6.23	1.16	1.23
1	B	24	THR	C-O	-6.23	1.16	1.24
1	D	275	ASP	C-O	-6.18	1.15	1.23
1	C	137	LEU	C-O	-5.65	1.17	1.24
1	B	23	SER	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	ASP	CG-OD2	-5.49	1.15	1.25
1	C	225	ILE	C-O	-5.43	1.18	1.24
1	D	265	TYR	C-O	-5.42	1.16	1.24
1	A	70	PHE	C-O	-5.38	1.16	1.23
1	B	149	LEU	C-O	-5.29	1.17	1.23
1	A	130	HIS	CG-ND1	-5.28	1.32	1.38
1	D	176	SER	C-O	-5.26	1.17	1.24
1	D	275	ASP	CB-CG	-5.21	1.39	1.52
1	A	16	LYS	CA-CB	-5.18	1.46	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	LYS	N-CA-C	9.66	124.88	112.89
1	B	117	GLU	N-CA-C	8.81	124.71	113.25
1	D	277	SER	N-CA-C	7.58	120.81	110.35
1	B	228	VAL	N-CA-C	7.43	119.96	108.44
1	C	266	VAL	CA-C-N	-6.54	114.07	122.77
1	C	266	VAL	C-N-CA	-6.54	114.07	122.77
1	D	274	PHE	N-CA-C	6.47	120.20	109.46
1	D	275	ASP	N-CA-CB	-6.11	102.01	110.38
1	A	91	GLY	N-CA-C	5.98	118.19	111.85
1	D	22	ASN	CA-C-O	5.73	126.00	119.18
1	D	49	ILE	CA-C-N	5.72	125.70	120.03
1	D	49	ILE	C-N-CA	5.72	125.70	120.03
1	D	132	GLU	N-CA-C	5.68	117.28	111.14
1	D	61	THR	CA-C-N	-5.49	113.96	119.56
1	D	61	THR	C-N-CA	-5.49	113.96	119.56
1	A	182	SER	N-CA-C	5.41	117.06	108.79
1	B	217	ASP	CA-C-N	5.36	125.43	119.32
1	B	217	ASP	C-N-CA	5.36	125.43	119.32
1	A	117	GLU	N-CA-C	5.29	121.51	109.81
1	B	244	LEU	N-CA-C	5.25	116.69	110.97
1	D	274	PHE	CA-C-O	5.19	126.40	120.54
1	A	272	HIS	N-CA-C	5.13	117.66	109.96
1	C	137	LEU	N-CA-C	-5.05	105.77	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	116	GLN	Peptide

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	2270	0	2167	56	0
1	B	2270	0	2165	36	0
1	C	2261	0	2154	36	0
1	D	2262	0	2157	47	0
2	A	48	0	0	3	0
2	B	45	0	0	3	0
2	C	40	0	0	0	0
2	D	50	0	0	2	0
All	All	9246	0	8643	165	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 9.

All (165) 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:68:LYS:HE2	2:B:341:HOH:O	1.56	1.05
1:A:190:VAL:CG2	1:A:253:LEU:HB2	1.86	1.04
1:A:190:VAL:HG21	1:A:253:LEU:HB2	1.00	0.97
1:A:190:VAL:HG21	1:A:253:LEU:CB	1.96	0.92
1:D:271:VAL:HG12	1:D:274:PHE:HD2	1.37	0.90
1:D:271:VAL:HG12	1:D:274:PHE:CD2	2.08	0.89
1:B:28:MET:HE1	1:B:89:PRO:HA	1.54	0.88
1:A:214:GLU:HG2	1:A:220:LEU:HD13	1.57	0.85
1:A:16:LYS:HG2	1:A:31:ASN:OD1	1.77	0.84
1:A:158:THR:HG22	1:A:159:GLY:H	1.45	0.82
1:C:290:GLU:O	1:C:294:ARG:HG3	1.80	0.82
1:A:61:THR:HG22	1:A:63:ASP:H	1.45	0.81
1:A:70:PHE:HB2	1:B:70:PHE:CZ	2.19	0.78
1:D:158:THR:HG22	1:D:159:GLY:H	1.48	0.77
1:A:61:THR:HG23	1:A:62:PRO:HD2	1.69	0.75
1:B:1:MET:HE2	1:B:140:HIS:HB3	1.69	0.74
1:D:117:GLU:N	1:D:118:PRO:HD2	2.03	0.73
1:D:158:THR:HG22	1:D:159:GLY:N	2.01	0.73
1:A:182:SER:HB2	1:A:295:ASN:HD22	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE1	1:B:137:LEU:HA	1.71	0.72
1:B:227:HIS:O	1:B:228:VAL:HG13	1.91	0.70
1:A:158:THR:HG22	1:A:159:GLY:N	2.08	0.69
1:D:175:TYR:CE1	1:D:178:LYS:HE2	2.28	0.69
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.06	0.68
1:C:222:ILE:HD13	1:C:257:VAL:CG1	2.24	0.68
1:B:263:GLN:O	1:B:264:ASP:HB2	1.94	0.67
1:C:5:LYS:HD2	1:C:6:GLU:H	1.59	0.67
1:A:271:VAL:HG21	1:A:284:PHE:CZ	2.29	0.67
1:D:158:THR:CG2	1:D:159:GLY:H	2.08	0.65
1:B:28:MET:CE	1:B:89:PRO:HA	2.26	0.65
1:D:214:GLU:HG2	1:D:220:LEU:HD13	1.81	0.62
1:C:1:MET:HG3	1:C:19:HIS:HB3	1.79	0.62
1:A:93:GLU:H	1:A:93:GLU:CD	2.08	0.62
1:D:271:VAL:CG1	1:D:274:PHE:CD2	2.83	0.62
1:D:263:GLN:O	1:D:264:ASP:HB2	2.00	0.61
1:A:6:GLU:OE2	1:A:13:ARG:NH1	2.34	0.61
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.65	0.61
1:D:68:LYS:HB3	1:D:278:TYR:HB3	1.82	0.60
1:A:190:VAL:HG22	1:A:219:CYS:SG	2.42	0.60
1:B:52:VAL:HG22	1:B:156:ALA:HB3	1.84	0.60
1:B:153:ASP:O	1:B:181:LYS:HE2	2.02	0.60
1:C:117:GLU:HB3	1:C:118:PRO:HA	1.82	0.60
1:D:158:THR:CG2	1:D:159:GLY:N	2.65	0.60
1:D:113:ASN:HD21	1:D:127:ASP:H	1.50	0.59
1:D:173:LYS:N	1:D:174:GLY:HA3	2.17	0.59
1:D:238:GLY:HA3	1:D:274:PHE:O	2.02	0.59
1:C:6:GLU:OE2	1:C:13:ARG:NH1	2.35	0.59
1:C:1:MET:HE3	1:C:17:LEU:HD13	1.83	0.59
1:C:221:LEU:O	1:C:225:ILE:HD12	2.04	0.58
1:B:254:LEU:HD12	1:B:268:ILE:HD12	1.84	0.58
1:B:26:THR:HG22	1:B:28:MET:HE3	1.84	0.57
1:D:117:GLU:N	1:D:118:PRO:CD	2.67	0.57
1:B:62:PRO:HB3	1:B:84:PHE:O	2.05	0.57
1:A:16:LYS:HE2	1:A:63:ASP:OD1	2.05	0.56
1:A:182:SER:CB	1:A:295:ASN:HD22	2.19	0.56
1:B:1:MET:HE2	1:B:140:HIS:CB	2.35	0.56
1:B:214:GLU:HG3	1:B:220:LEU:HD13	1.88	0.56
1:B:50:PRO:HB2	1:B:296:LEU:HD13	1.87	0.56
1:A:70:PHE:HB2	1:B:70:PHE:CE1	2.42	0.55
1:C:1:MET:HE1	1:C:137:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:HD21	1:A:149:LEU:H	1.55	0.54
1:A:128:TYR:HD2	1:A:129:ILE:HD12	1.73	0.54
1:D:75:ALA:HB1	1:D:80:PHE:O	2.08	0.54
1:D:191:ASN:HD22	1:D:252:LEU:HD13	1.73	0.54
1:B:86:ASP:OD2	1:B:90:ARG:HD2	2.08	0.53
1:B:26:THR:CG2	1:B:28:MET:HE3	2.39	0.53
1:B:62:PRO:HD3	1:B:86:ASP:HA	1.91	0.53
1:D:227:HIS:HB3	1:D:261:SER:HB2	1.90	0.52
1:A:260:THR:HG22	1:A:261:SER:N	2.25	0.52
1:B:67:GLU:HG2	2:B:301:HOH:O	2.09	0.52
1:D:214:GLU:CG	1:D:220:LEU:HD13	2.40	0.52
1:B:1:MET:HE1	1:B:137:LEU:HD23	1.91	0.52
1:D:236:HIS:HD2	1:D:288:HIS:NE2	2.08	0.51
1:A:1:MET:HE2	1:A:140:HIS:CB	2.39	0.51
1:D:116:GLN:C	1:D:118:PRO:HD2	2.35	0.51
1:D:190:VAL:CG1	1:D:253:LEU:HB2	2.41	0.51
1:A:236:HIS:HD2	1:A:288:HIS:NE2	2.08	0.51
1:C:1:MET:HE2	1:C:140:HIS:CG	2.46	0.51
1:A:158:THR:CG2	1:A:159:GLY:H	2.21	0.51
1:D:130:HIS:ND1	1:D:180:TYR:OH	2.39	0.51
1:A:1:MET:HE2	1:A:140:HIS:CG	2.46	0.50
1:A:283:THR:HG23	1:B:10:CYS:HA	1.93	0.50
1:D:24:THR:HG23	1:D:89:PRO:HB3	1.92	0.50
1:B:36:LYS:HG2	1:B:37:HIS:CD2	2.46	0.50
1:A:260:THR:HG22	1:A:262:TRP:H	1.77	0.50
1:C:182:SER:HB3	1:C:295:ASN:HD22	1.76	0.50
1:D:217:ASP:HB3	1:D:220:LEU:HD12	1.94	0.50
1:C:10:CYS:HA	1:D:283:THR:HG23	1.92	0.50
1:A:10:CYS:HA	1:B:283:THR:HG23	1.93	0.49
1:C:118:PRO:HD2	1:C:119:TYR:CE1	2.47	0.49
1:A:258:LYS:HA	1:A:263:GLN:HG3	1.94	0.49
1:A:294:ARG:CG	1:A:294:ARG:NH1	2.68	0.49
1:C:281:VAL:O	1:C:285:VAL:HG23	2.12	0.49
1:B:14:LEU:HD12	1:B:33:TYR:HB2	1.93	0.49
1:A:15:ILE:HG22	1:A:17:LEU:HG	1.94	0.49
1:C:33:TYR:CE2	1:C:35:PRO:HA	2.47	0.48
1:B:61:THR:HB	1:B:62:PRO:HD2	1.94	0.48
1:D:26:THR:HG22	1:D:27:SER:N	2.28	0.48
1:A:64:ASN:O	1:A:68:LYS:HG3	2.13	0.48
1:C:275:ASP:OD2	1:D:7:PHE:HD2	1.96	0.48
1:C:108:ALA:HA	1:C:162:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLU:OE1	1:C:258:LYS:HD2	2.13	0.48
1:C:294:ARG:HG2	1:C:299:ILE:HD11	1.95	0.47
1:D:154:ASN:HB2	1:D:181:LYS:HG3	1.97	0.47
1:B:26:THR:HG22	1:B:27:SER:O	2.14	0.47
1:D:271:VAL:HG12	1:D:274:PHE:CE2	2.50	0.47
1:D:271:VAL:CG1	1:D:274:PHE:CE2	2.99	0.46
1:C:61:THR:H	1:C:64:ASN:ND2	2.13	0.46
1:D:184:SER:OG	1:D:288:HIS:ND1	2.47	0.46
1:A:279:TYR:HB3	1:B:9:VAL:HG22	1.97	0.46
1:A:58:LEU:HD22	1:A:103:ASP:HA	1.97	0.46
1:A:101:SER:HB3	1:C:99:GLU:HB3	1.98	0.46
1:C:93:GLU:H	1:C:93:GLU:CD	2.24	0.46
1:A:275:ASP:HB2	2:A:348:HOH:O	2.15	0.46
1:A:70:PHE:CE2	1:A:73:PHE:HB2	2.51	0.46
1:A:275:ASP:HB3	1:A:277:SER:H	1.80	0.45
1:C:222:ILE:HD13	1:C:257:VAL:HG11	1.98	0.45
1:C:222:ILE:HD13	1:C:257:VAL:HG12	1.95	0.45
1:A:192:PRO:HB2	1:A:202:PHE:CE1	2.52	0.45
1:D:190:VAL:HG22	1:D:253:LEU:HD22	1.98	0.45
1:D:49:ILE:HA	1:D:50:PRO:HD3	1.83	0.45
1:D:118:PRO:HG2	1:D:119:TYR:CD1	2.51	0.45
1:D:190:VAL:HG11	1:D:253:LEU:HB2	1.98	0.45
1:D:254:LEU:HD23	1:D:268:ILE:HD12	1.99	0.44
1:B:202:PHE:HB3	1:B:213:TRP:CE2	2.53	0.44
1:B:75:ALA:HB1	1:B:80:PHE:O	2.18	0.44
1:C:239:ASP:OD2	1:C:272:HIS:HA	2.17	0.44
1:A:1:MET:HE2	1:A:140:HIS:HB3	2.00	0.44
1:A:70:PHE:HB2	1:B:70:PHE:CE2	2.53	0.44
1:C:49:ILE:HA	1:C:50:PRO:HD3	1.88	0.44
1:C:24:THR:HA	1:C:122:HIS:O	2.18	0.43
1:A:236:HIS:CD2	1:A:288:HIS:NE2	2.85	0.43
1:B:275:ASP:HB3	1:B:277:SER:H	1.83	0.43
1:D:68:LYS:HB3	1:D:278:TYR:CB	2.47	0.43
1:A:129:ILE:HG22	1:A:130:HIS:CG	2.53	0.43
1:A:245:GLU:O	1:A:249:LYS:HE2	2.19	0.43
1:B:30:VAL:HG22	2:B:314:HOH:O	2.19	0.43
1:A:236:HIS:HE1	2:A:325:HOH:O	2.01	0.43
1:C:214:GLU:HA	1:C:220:LEU:HD12	1.99	0.43
1:D:165:TYR:HB2	1:D:189:ILE:O	2.19	0.43
1:D:202:PHE:HB3	1:D:213:TRP:CE2	2.54	0.43
1:C:61:THR:HB	1:C:62:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LEU:HD23	1:C:266:VAL:HG11	2.00	0.42
1:C:244:LEU:O	1:C:245:GLU:CB	2.66	0.42
1:A:202:PHE:HB3	1:A:213:TRP:CE2	2.55	0.42
1:C:61:THR:HB	1:C:62:PRO:HD2	2.01	0.42
1:B:6:GLU:HG2	1:B:15:ILE:HG12	2.02	0.42
1:B:19:HIS:HE1	1:B:128:TYR:OH	2.03	0.42
1:C:97:ASP:HA	1:C:98:PRO:HD3	1.91	0.42
1:C:103:ASP:OD1	1:C:197:TRP:CD1	2.73	0.42
1:D:213:TRP:HB2	2:D:331:HOH:O	2.19	0.42
1:C:1:MET:SD	1:C:136:THR:HG22	2.60	0.41
1:D:97:ASP:HA	1:D:98:PRO:HD3	1.95	0.41
1:A:104:PHE:CB	1:A:200:LYS:HE2	2.51	0.41
1:C:161:SER:HA	1:C:187:ALA:O	2.20	0.41
1:A:61:THR:HG23	1:A:62:PRO:CD	2.46	0.41
1:A:271:VAL:HG21	1:A:284:PHE:HZ	1.80	0.41
1:D:37:HIS:H	1:D:37:HIS:CD2	2.38	0.41
1:D:64:ASN:HB2	2:D:310:HOH:O	2.20	0.41
1:A:270:LYS:HD3	2:A:316:HOH:O	2.21	0.41
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.92	0.40
1:D:244:LEU:HD12	1:D:250:PRO:HD3	2.03	0.40
1:A:7:PHE:CD2	1:B:275:ASP:OD2	2.75	0.40
1:D:34:LEU:HA	1:D:35:PRO:HD2	1.95	0.40
1:A:138:ASP:O	1:A:142:ASN:HB2	2.20	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	275/299 (92%)	262 (95%)	13 (5%)	0	100	100
1	B	275/299 (92%)	260 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	274/299 (92%)	259 (94%)	14 (5%)	1 (0%)	30	23
1	D	275/299 (92%)	263 (96%)	12 (4%)	0	100	100
All	All	1099/1196 (92%)	1044 (95%)	54 (5%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	245	GLU

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	241/255 (94%)	233 (97%)	8 (3%)	33	28
1	B	241/255 (94%)	236 (98%)	5 (2%)	47	45
1	C	240/255 (94%)	237 (99%)	3 (1%)	61	62
1	D	241/255 (94%)	236 (98%)	5 (2%)	47	45
All	All	963/1020 (94%)	942 (98%)	21 (2%)	45	43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	61	THR
1	A	101	SER
1	A	129	ILE
1	A	152	LEU
1	A	160	ILE
1	A	263	GLN
1	A	294	ARG
1	B	1	MET
1	B	26	THR
1	B	189	ILE

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Mol	Chain	Res	Type
1	B	248	LEU
1	B	251	GLU
1	C	190	VAL
1	C	223	LYS
1	C	232	ARG
1	D	9	VAL
1	D	68	LYS
1	D	190	VAL
1	D	254	LEU
1	D	275	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	140	HIS
1	A	142	ASN
1	A	236	HIS
1	A	295	ASN
1	B	19	HIS
1	B	29	ASN
1	B	37	HIS
1	B	74	GLN
1	B	154	ASN
1	B	191	ASN
1	B	194	ASN
1	C	19	HIS
1	C	29	ASN
1	C	64	ASN
1	C	130	HIS
1	C	199	GLN
1	C	227	HIS
1	C	295	ASN
1	D	19	HIS
1	D	113	ASN
1	D	116	GLN
1	D	122	HIS
1	D	191	ASN
1	D	236	HIS

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](#)

There are no ligands in this entry.

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	283/299 (94%)	0.60	8 (2%) 55 56	8, 13, 21, 31	0
1	B	283/299 (94%)	0.41	5 (1%) 67 69	7, 12, 20, 24	0
1	C	282/299 (94%)	0.92	27 (9%) 13 14	9, 18, 31, 35	0
1	D	282/299 (94%)	0.52	9 (3%) 50 50	8, 12, 20, 28	1 (0%)
All	All	1130/1196 (94%)	0.61	49 (4%) 40 40	7, 14, 24, 35	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	4.5
1	A	117	GLU	4.4
1	C	93	GLU	3.4
1	D	118	PRO	3.2
1	C	252	LEU	3.1
1	C	250	PRO	3.1
1	D	92	ASP	3.1
1	C	258	LYS	3.1
1	A	118	PRO	3.0
1	C	95	ALA	2.9
1	B	117	GLU	2.7
1	D	117	GLU	2.7
1	C	206	LEU	2.7
1	C	161	SER	2.7
1	D	271	VAL	2.6
1	C	213	TRP	2.6
1	C	103	ASP	2.6
1	C	271	VAL	2.5
1	A	248	LEU	2.5
1	C	228	VAL	2.5
1	D	248	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	228	VAL	2.4
1	B	207	GLY	2.4
1	A	245	GLU	2.4
1	C	94	VAL	2.4
1	C	259	ALA	2.3
1	B	7	PHE	2.3
1	C	9	VAL	2.3
1	C	176	SER	2.3
1	C	230	ASP	2.3
1	A	7	PHE	2.3
1	C	220	LEU	2.3
1	D	254	LEU	2.2
1	A	41	GLN	2.2
1	A	2	LYS	2.2
1	C	40	ALA	2.2
1	C	294	ARG	2.2
1	A	3	VAL	2.2
1	C	114	ALA	2.1
1	B	275	ASP	2.1
1	C	118	PRO	2.1
1	C	297	GLY	2.1
1	C	226	ARG	2.1
1	C	249	LYS	2.1
1	C	254	LEU	2.1
1	D	121	GLN	2.0
1	B	118	PRO	2.0
1	C	5	LYS	2.0
1	D	207	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.