



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 PM UTC

PDB ID : 4X9E / pdb_00004x9e
Title : DEOXYGUANOSINETRIPHOSPHATE TRIPHOSPHOHYDROLASE from
Escherichia coli with two DNA effector molecules
Authors : Singh, D.; Gawel, D.; Itsko, M.; Krahn, J.M.; London, R.E.; Schaaper, R.M.
Deposited on : 2014-12-11
Resolution : 3.10 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

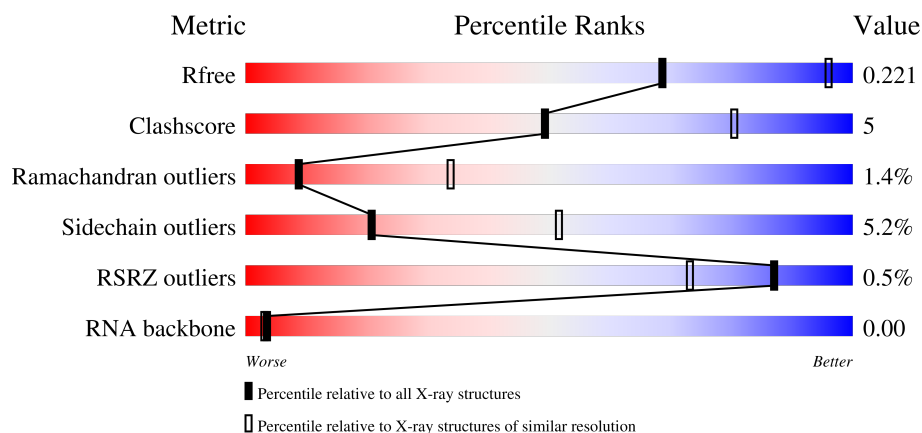
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	505	76% 21% ..
1	B	505	80% 16% ..
1	C	505	81% 16% ..
1	D	505	81% 15% ..

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Mol	Chain	Length	Quality of chain
1	E	505	81% 15%
1	F	505	83% 12%
2	G	3	67% 33%
2	H	3	33% 67% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24471 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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4092	2618	728	730	16			
1	B	495	Total	C	N	O	S	0	0	0
			3983	2562	709	696	16			
1	C	500	Total	C	N	O	S	0	0	0
			4107	2627	730	733	17			
1	D	501	Total	C	N	O	S	0	0	0
			4067	2606	713	732	16			
1	E	496	Total	C	N	O	S	0	0	0
			4075	2609	715	735	16			
1	F	497	Total	C	N	O	S	0	0	0
			4034	2588	715	715	16			

- Molecule 2 is a RNA chain called RNA (5'-R(P*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	P	0	0	0
			58	27	9	19	3			
2	H	3	Total	C	N	O	P	0	0	0
			53	27	9	15	2			

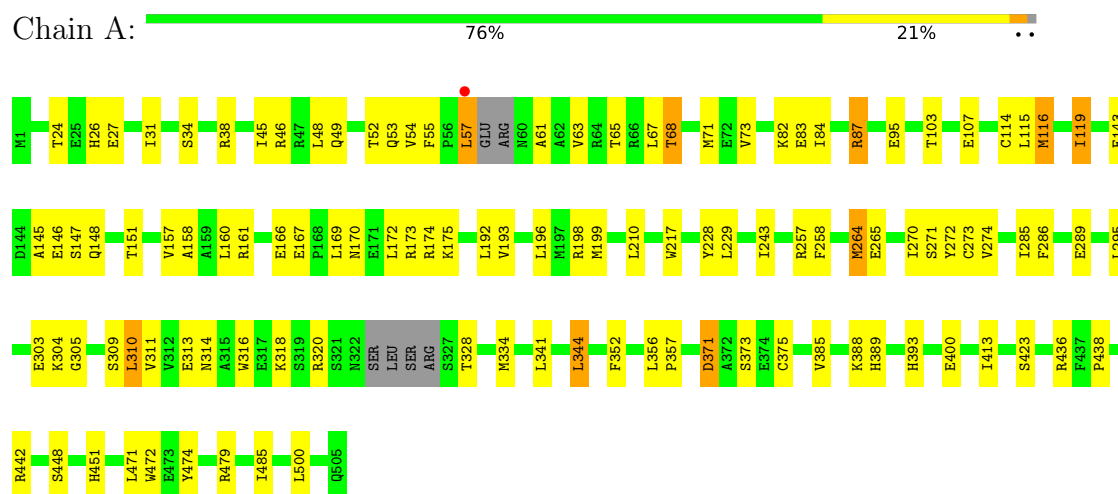
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

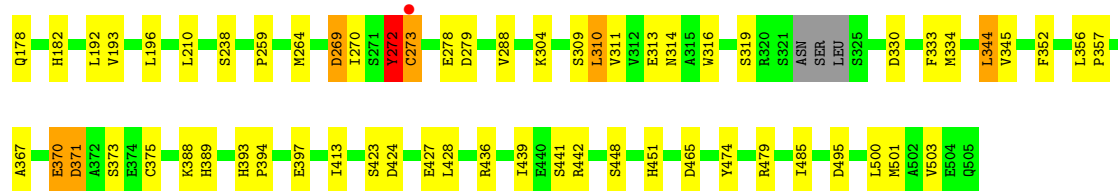
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

3 Residue-property plots [i](#)

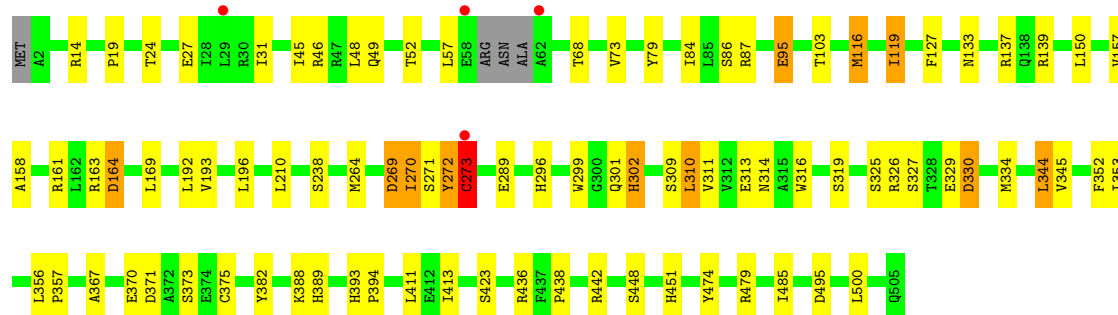
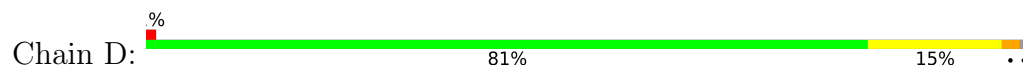
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Deoxyguanosinetriphosphate triphosphohydrolase

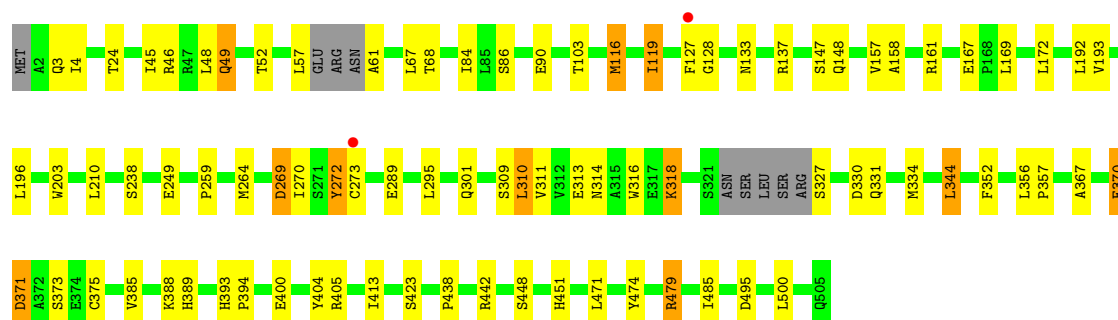
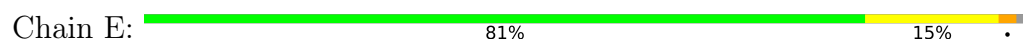




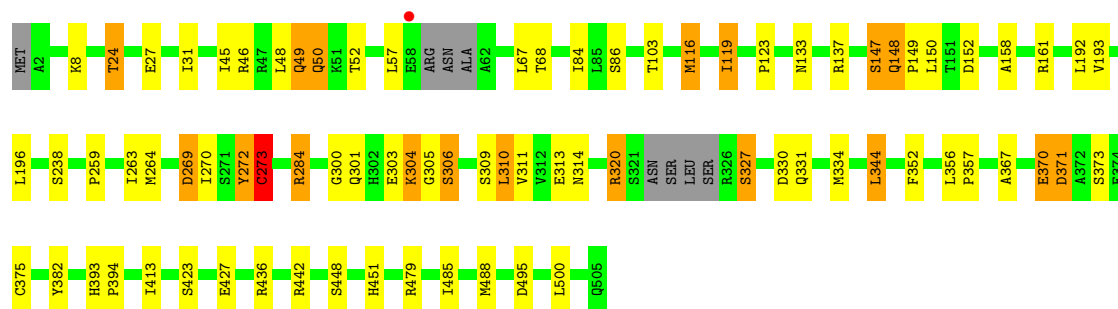
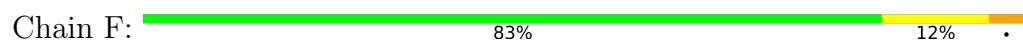
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



• Molecule 2: RNA (5'-R(P*CP*CP*C)-3')

Chain G:  67% 33%



● Molecule 2: RNA (5'-R(P*CP*CP*C)-3')

Chain H:  33% 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.80Å 159.80Å 190.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.10 49.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.63-3.10) 95.8 (49.63-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.167 , 0.223 0.170 , 0.221	Depositor DCC
R_{free} test set	3881 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24471	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: MG

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	0/4193	0.91	3/5674 (0.1%)
1	B	0.54	0/4083	0.88	5/5532 (0.1%)
1	C	0.69	5/4208 (0.1%)	0.92	5/5692 (0.1%)
1	D	0.62	3/4169 (0.1%)	0.88	1/5649 (0.0%)
1	E	0.69	3/4176 (0.1%)	0.91	4/5651 (0.1%)
1	F	0.63	4/4134 (0.1%)	0.91	8/5599 (0.1%)
2	G	0.42	0/63	0.36	0/92
2	H	0.33	0/58	0.34	0/87
All	All	0.63	15/25084 (0.1%)	0.90	26/33976 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	270	ILE	C-O	7.06	1.32	1.24
1	F	270	ILE	C-O	6.91	1.32	1.24
1	E	270	ILE	C-O	6.39	1.31	1.24
1	C	270	ILE	C-O	6.38	1.31	1.24
1	F	269	ASP	C-O	6.19	1.31	1.24
1	C	259	PRO	C-O	5.73	1.31	1.24
1	C	273	CYS	C-O	5.73	1.30	1.24
1	C	269	ASP	C-O	5.50	1.30	1.24
1	D	273	CYS	C-O	5.27	1.30	1.24
1	D	269	ASP	C-O	5.26	1.30	1.24
1	E	259	PRO	C-O	5.25	1.30	1.24
1	F	273	CYS	C-O	5.20	1.30	1.24
1	C	272	TYR	C-O	5.19	1.30	1.24
1	F	259	PRO	C-O	5.12	1.30	1.24
1	E	269	ASP	C-O	5.08	1.30	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	148	GLN	CA-C-N	7.99	129.82	119.84
1	F	148	GLN	C-N-CA	7.99	129.82	119.84
1	F	305	GLY	N-CA-C	-7.49	106.16	115.08
1	C	167	GLU	CA-C-N	-6.09	112.21	118.85
1	C	167	GLU	C-N-CA	-6.09	112.21	118.85
1	A	116	MET	N-CA-C	5.78	118.28	110.88
1	D	116	MET	N-CA-C	5.72	118.20	110.88
1	B	116	MET	N-CA-C	5.70	118.17	110.88
1	E	116	MET	N-CA-C	5.62	118.07	110.88
1	C	116	MET	N-CA-C	5.61	118.05	110.88
1	F	116	MET	N-CA-C	5.53	117.96	110.88
1	C	49	GLN	CA-C-N	-5.36	114.14	122.67
1	C	49	GLN	C-N-CA	-5.36	114.14	122.67
1	E	128	GLY	N-CA-C	-5.30	106.35	112.50
1	F	263	ILE	N-CA-C	5.23	115.44	110.42
1	E	49	GLN	CA-C-N	-5.18	114.43	122.67
1	E	49	GLN	C-N-CA	-5.18	114.43	122.67
1	A	258	PHE	CA-C-N	5.18	126.31	119.84
1	A	258	PHE	C-N-CA	5.18	126.31	119.84
1	B	258	PHE	CA-C-N	5.13	126.26	119.84
1	B	258	PHE	C-N-CA	5.13	126.26	119.84
1	F	50	GLN	N-CA-C	5.10	118.81	112.59
1	F	49	GLN	CA-C-N	-5.09	114.58	122.67
1	F	49	GLN	C-N-CA	-5.09	114.58	122.67
1	B	285	ILE	N-CA-C	5.03	115.75	110.62
1	B	272	TYR	N-CA-C	-5.02	105.81	111.28

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	4092	0	4021	61	1
1	B	3983	0	3877	46	0
1	C	4107	0	4033	44	1
1	D	4067	0	3945	47	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4075	0	3997	44	0
1	F	4034	0	3941	38	1
2	G	58	0	34	1	0
2	H	53	0	32	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	24471	0	23880	263	2

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 5.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ALA:HB2	1:F:50:GLN:HG3	1.52	0.91
1:E:371:ASP:HB3	1:E:373:SER:H	1.48	0.79
1:F:371:ASP:HB3	1:F:373:SER:H	1.48	0.79
1:B:371:ASP:HB3	1:B:373:SER:H	1.49	0.78
1:D:371:ASP:HB3	1:D:373:SER:H	1.48	0.78
1:C:371:ASP:HB3	1:C:373:SER:H	1.48	0.76
1:A:371:ASP:HB3	1:A:373:SER:H	1.51	0.74
1:C:442:ARG:CZ	1:E:127:PHE:HZ	2.01	0.73
1:C:310:LEU:O	1:C:314:ASN:HB3	1.90	0.72
1:D:310:LEU:O	1:D:314:ASN:HB3	1.90	0.72
1:A:289:GLU:HG3	1:A:316:TRP:HH2	1.55	0.72
1:E:310:LEU:O	1:E:314:ASN:HB3	1.91	0.71
1:F:310:LEU:O	1:F:314:ASN:HB3	1.91	0.71
1:F:284:ARG:HA	1:F:284:ARG:HH11	1.56	0.70
1:A:57:LEU:HD22	1:A:65:THR:HG22	1.73	0.69
1:B:413:ILE:HG21	1:B:500:LEU:HD13	1.75	0.69
1:D:119:ILE:HG23	1:D:192:LEU:HD23	1.76	0.68
1:A:310:LEU:O	1:A:314:ASN:HB3	1.93	0.68
1:F:367:ALA:HB3	1:F:370:GLU:HB3	1.75	0.68
1:B:310:LEU:O	1:B:314:ASN:HB3	1.93	0.67
1:F:119:ILE:HG23	1:F:192:LEU:HD23	1.77	0.67
1:E:367:ALA:HB3	1:E:370:GLU:HB3	1.76	0.67
1:A:68:THR:HG21	1:B:46:ARG:HG2	1.77	0.67
1:C:367:ALA:HB3	1:C:370:GLU:HB3	1.76	0.67
1:E:119:ILE:HG23	1:E:192:LEU:HD23	1.77	0.66
1:C:119:ILE:HG23	1:C:192:LEU:HD23	1.78	0.65
1:D:299:TRP:HD1	1:D:302:HIS:HD1	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ALA:HB3	1:D:370:GLU:HB3	1.78	0.65
1:A:119:ILE:HG23	1:A:192:LEU:HD23	1.78	0.64
1:D:161:ARG:HD2	1:D:163:ARG:HH22	1.61	0.64
1:B:119:ILE:HG23	1:B:192:LEU:HD23	1.79	0.64
1:A:229:LEU:HD22	1:A:257:ARG:HD3	1.78	0.64
1:D:299:TRP:HD1	1:D:302:HIS:ND1	1.96	0.64
1:D:95:GLU:CD	1:D:95:GLU:H	2.05	0.64
1:A:413:ILE:HG21	1:A:500:LEU:HD13	1.80	0.63
1:A:45:ILE:O	1:A:48:LEU:HB2	2.00	0.62
1:A:46:ARG:HG2	1:B:68:THR:HG21	1.81	0.62
1:D:164:ASP:OD1	1:D:164:ASP:N	2.32	0.62
1:B:400:GLU:OE1	1:D:442:ARG:NE	2.32	0.62
1:B:229:LEU:HD22	1:B:257:ARG:HD3	1.81	0.62
1:D:299:TRP:CD1	1:D:302:HIS:HD1	2.19	0.60
1:C:448:SER:HB2	1:C:451:HIS:CD2	2.37	0.60
1:A:82:LYS:HE2	1:A:107:GLU:OE1	2.01	0.60
1:C:288:VAL:HG12	1:C:316:TRP:HZ3	1.67	0.60
1:B:45:ILE:O	1:B:48:LEU:HB2	2.01	0.59
1:C:393:HIS:CD2	1:C:394:PRO:HD2	2.37	0.59
1:D:45:ILE:O	1:D:48:LEU:HB2	2.03	0.59
1:D:289:GLU:HG3	1:D:316:TRP:HH2	1.67	0.58
1:E:158:ALA:HA	1:E:161:ARG:HH12	1.69	0.58
1:E:413:ILE:HG21	1:E:500:LEU:HD13	1.85	0.58
1:E:448:SER:HB2	1:E:451:HIS:CD2	2.39	0.58
1:D:87:ARG:HD3	1:D:353:ILE:HD12	1.86	0.57
1:F:413:ILE:HG21	1:F:500:LEU:HD13	1.86	0.57
1:A:158:ALA:HA	1:A:161:ARG:NH1	2.20	0.56
1:D:413:ILE:HG21	1:D:500:LEU:HD13	1.87	0.56
1:F:393:HIS:CD2	1:F:394:PRO:HD2	2.41	0.56
1:C:439:ILE:HD11	1:E:404:TYR:CD1	2.41	0.55
1:A:438:PRO:O	1:A:442:ARG:HG3	2.06	0.55
1:B:49:GLN:HB3	1:B:67:LEU:HD22	1.88	0.55
1:E:3:GLN:OE1	1:E:4:ILE:N	2.38	0.55
1:C:413:ILE:HG21	1:C:500:LEU:HD13	1.88	0.55
1:E:344:LEU:HD22	1:E:375:CYS:HB3	1.90	0.54
1:F:45:ILE:O	1:F:48:LEU:HB2	2.07	0.54
1:A:49:GLN:HB3	1:A:67:LEU:HD22	1.89	0.54
1:F:427:GLU:CD	1:F:436:ARG:HH22	2.16	0.54
1:A:160:LEU:HD23	1:A:471:LEU:HD22	1.89	0.54
1:D:84:ILE:HD13	1:D:352:PHE:CD2	2.43	0.53
1:C:84:ILE:HD13	1:C:352:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:SER:HB2	1:D:451:HIS:CD2	2.44	0.53
1:C:424:ASP:OD1	1:C:436:ARG:NH2	2.42	0.53
1:E:84:ILE:HD13	1:E:352:PHE:CD2	2.44	0.53
1:E:45:ILE:O	1:E:48:LEU:HB2	2.08	0.53
1:C:64:ARG:NH1	1:C:279:ASP:OD1	2.42	0.52
1:A:145:ALA:O	1:A:174:ARG:HG2	2.10	0.52
1:A:175:LYS:HG2	1:A:217:TRP:CD1	2.44	0.52
1:F:84:ILE:HD13	1:F:352:PHE:CD2	2.44	0.52
1:A:303:GLU:O	1:A:305:GLY:N	2.42	0.52
1:C:45:ILE:O	1:C:48:LEU:HB2	2.07	0.52
1:B:448:SER:HB2	1:B:451:HIS:CD2	2.45	0.52
1:E:133:ASN:O	1:E:137:ARG:HB2	2.09	0.52
1:E:46:ARG:O	1:E:49:GLN:HG2	2.10	0.52
1:E:158:ALA:HA	1:E:161:ARG:NH1	2.25	0.52
1:C:158:ALA:HA	1:C:161:ARG:HH12	1.75	0.51
1:A:270:ILE:HG21	1:A:341:LEU:CD2	2.40	0.51
1:A:448:SER:HB2	1:A:451:HIS:CD2	2.46	0.51
1:E:314:ASN:O	1:E:318:LYS:HB2	2.09	0.51
1:B:160:LEU:HD23	1:B:471:LEU:HD22	1.91	0.51
1:B:175:LYS:HG2	1:B:217:TRP:CD1	2.46	0.51
1:C:393:HIS:CG	1:C:394:PRO:HD2	2.46	0.51
1:C:442:ARG:NH1	1:E:127:PHE:HZ	2.08	0.51
1:F:448:SER:HB2	1:F:451:HIS:CD2	2.44	0.51
1:B:158:ALA:HA	1:B:161:ARG:NH1	2.26	0.51
1:C:269:ASP:O	1:C:272:TYR:HB3	2.10	0.50
1:B:285:ILE:HG23	1:B:393:HIS:HD2	1.74	0.50
1:F:344:LEU:HD22	1:F:375:CYS:HB3	1.93	0.50
1:A:228:TYR:OH	1:A:265:GLU:OE1	2.28	0.50
1:B:270:ILE:HG21	1:B:341:LEU:CD2	2.41	0.50
1:F:269:ASP:O	1:F:272:TYR:HB3	2.11	0.50
1:F:303:GLU:O	1:F:306:SER:HB3	2.12	0.50
1:A:116:MET:HB2	1:A:119:ILE:HD12	1.94	0.50
1:E:393:HIS:CD2	1:E:394:PRO:HD2	2.47	0.49
1:A:27:GLU:O	1:A:31:ILE:HG13	2.12	0.49
1:A:289:GLU:HG3	1:A:316:TRP:CH2	2.42	0.49
1:D:46:ARG:O	1:D:49:GLN:HG2	2.12	0.49
1:A:71:MET:HE1	1:B:115:LEU:HD11	1.95	0.49
1:C:442:ARG:CZ	1:E:127:PHE:CZ	2.90	0.49
1:C:442:ARG:NE	1:E:400:GLU:OE1	2.39	0.49
1:D:158:ALA:HA	1:D:161:ARG:HH12	1.77	0.49
1:D:344:LEU:HD22	1:D:375:CYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD23	1:B:67:LEU:HD23	1.94	0.48
1:A:199:MET:HE2	1:A:199:MET:HB3	1.69	0.48
1:B:228:TYR:OH	1:B:265:GLU:OE1	2.30	0.48
1:B:84:ILE:HD13	1:B:352:PHE:CD2	2.48	0.48
1:C:46:ARG:O	1:C:49:GLN:HG2	2.13	0.48
1:C:344:LEU:HD22	1:C:375:CYS:HB3	1.95	0.48
1:D:158:ALA:HA	1:D:161:ARG:NH1	2.29	0.48
1:F:123:PRO:HG3	1:F:488:MET:O	2.14	0.48
1:A:115:LEU:HD11	1:B:71:MET:HE1	1.95	0.48
1:B:270:ILE:HG21	1:B:341:LEU:HD23	1.95	0.48
1:C:158:ALA:HA	1:C:161:ARG:NH1	2.28	0.48
1:E:388:LYS:HB3	1:E:389:HIS:CD2	2.49	0.48
1:B:388:LYS:HB3	1:B:389:HIS:CD2	2.48	0.47
1:F:133:ASN:O	1:F:137:ARG:HB2	2.15	0.47
1:C:133:ASN:O	1:C:137:ARG:HB2	2.15	0.47
1:E:147:SER:OG	1:E:148:GLN:N	2.46	0.47
1:F:158:ALA:HA	1:F:161:ARG:HH12	1.79	0.47
1:E:269:ASP:O	1:E:272:TYR:HB3	2.14	0.47
1:D:269:ASP:O	1:D:272:TYR:HB3	2.13	0.47
1:D:393:HIS:CD2	1:D:394:PRO:HD2	2.50	0.47
1:B:27:GLU:O	1:B:31:ILE:HG13	2.15	0.47
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.74	0.46
1:F:46:ARG:O	1:F:49:GLN:HG2	2.15	0.46
1:F:147:SER:HB3	1:F:148:GLN:H	1.50	0.46
1:A:172:LEU:HD23	1:A:471:LEU:HD12	1.96	0.46
1:A:273:CYS:SG	1:A:274:VAL:N	2.88	0.46
1:B:116:MET:HB2	1:B:119:ILE:HD12	1.96	0.46
1:E:289:GLU:HG3	1:E:316:TRP:HH2	1.81	0.46
1:A:73:VAL:HG12	1:A:114:CYS:HB3	1.98	0.46
1:D:192:LEU:HD12	1:D:196:LEU:HB2	1.98	0.46
1:D:388:LYS:HB3	1:D:389:HIS:CD2	2.51	0.46
1:F:393:HIS:CG	1:F:394:PRO:HD2	2.50	0.46
1:B:438:PRO:O	1:B:442:ARG:HG3	2.16	0.46
1:A:344:LEU:HD22	1:A:375:CYS:HB3	1.97	0.46
1:C:309:SER:O	1:C:313:GLU:HB3	2.16	0.46
1:A:84:ILE:HD13	1:A:352:PHE:CD2	2.52	0.45
1:D:289:GLU:HG3	1:D:316:TRP:CH2	2.49	0.45
1:C:157:VAL:HG21	1:C:474:TYR:CE2	2.52	0.45
1:A:388:LYS:HB3	1:A:389:HIS:CD2	2.51	0.45
1:F:116:MET:HB2	1:F:119:ILE:HD12	1.98	0.45
1:F:309:SER:O	1:F:313:GLU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ASN:O	1:D:137:ARG:HB2	2.17	0.45
1:E:116:MET:HB2	1:E:119:ILE:HD12	1.98	0.45
1:D:334:MET:HE2	1:D:334:MET:HB3	1.88	0.45
1:A:356:LEU:N	1:A:357:PRO:HD2	2.32	0.45
1:F:158:ALA:HA	1:F:161:ARG:NH1	2.32	0.45
1:B:172:LEU:HD23	1:B:471:LEU:HD12	2.00	0.44
1:A:53:GLN:HG3	1:A:54:VAL:HG23	1.99	0.44
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.76	0.44
1:C:178:GLN:O	1:C:182:HIS:HD2	2.00	0.44
1:D:116:MET:HB2	1:D:119:ILE:HD12	1.98	0.44
1:D:356:LEU:N	1:D:357:PRO:HD2	2.32	0.44
1:E:393:HIS:CG	1:E:394:PRO:HD2	2.52	0.44
1:C:501:MET:HA	1:E:405:ARG:HD2	1.99	0.44
1:A:158:ALA:HA	1:A:161:ARG:HH12	1.81	0.44
1:D:52:THR:HG22	1:D:57:LEU:HG	2.00	0.44
1:C:388:LYS:HB3	1:C:389:HIS:CD2	2.52	0.44
1:E:327:SER:O	1:E:331:GLN:HG2	2.18	0.44
1:A:166:GLU:O	1:A:170:ASN:ND2	2.50	0.44
1:B:344:LEU:HD22	1:B:375:CYS:HB3	1.99	0.44
1:D:27:GLU:O	1:D:31:ILE:HG13	2.17	0.44
1:E:309:SER:O	1:E:313:GLU:HB3	2.18	0.44
1:F:356:LEU:N	1:F:357:PRO:HD2	2.32	0.44
1:B:157:VAL:HG21	1:B:474:TYR:CE2	2.53	0.44
1:D:296:HIS:CD2	1:D:302:HIS:CE1	3.05	0.44
1:A:172:LEU:HD11	1:A:472:TRP:CZ2	2.53	0.44
1:B:309:SER:O	1:B:313:GLU:HB3	2.18	0.44
1:E:169:LEU:HD23	1:E:169:LEU:HA	1.84	0.44
1:A:243:ILE:HD13	1:A:243:ILE:HA	1.80	0.43
1:B:53:GLN:HG3	1:B:54:VAL:HG23	1.98	0.43
1:C:116:MET:HB2	1:C:119:ILE:HD12	1.99	0.43
1:C:356:LEU:N	1:C:357:PRO:HD2	2.32	0.43
1:A:320:ARG:HE	1:A:320:ARG:HB3	1.66	0.43
1:C:192:LEU:HD12	1:C:196:LEU:HB2	1.99	0.43
1:C:79:TYR:CD1	1:C:345:VAL:HG21	2.53	0.43
1:D:79:TYR:CD1	1:D:345:VAL:HG21	2.54	0.43
1:D:411:LEU:HD23	1:D:411:LEU:HA	1.89	0.43
1:A:270:ILE:HG21	1:A:341:LEU:HD23	2.00	0.43
1:A:400:GLU:OE1	1:E:442:ARG:NE	2.51	0.43
1:B:166:GLU:O	1:B:170:ASN:ND2	2.51	0.43
1:F:150:LEU:C	1:F:152:ASP:H	2.27	0.43
1:F:192:LEU:HD12	1:F:196:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:O	1:A:87:ARG:HB2	2.19	0.43
1:C:52:THR:HG22	1:C:57:LEU:HG	2.01	0.43
1:F:334:MET:HE2	1:F:334:MET:HB3	1.91	0.43
1:C:147:SER:OG	1:C:148:GLN:N	2.43	0.43
1:A:46:ARG:O	1:A:49:GLN:HG2	2.19	0.43
1:B:295:LEU:HD23	1:B:385:VAL:HG21	2.01	0.43
1:E:67:LEU:HD23	1:F:67:LEU:HD23	2.00	0.43
1:A:46:ARG:O	1:A:49:GLN:N	2.52	0.43
1:E:203:TRP:CE2	1:E:249:GLU:HG3	2.54	0.43
1:F:27:GLU:O	1:F:31:ILE:HG13	2.19	0.43
1:E:356:LEU:N	1:E:357:PRO:HD2	2.34	0.43
1:A:38:ARG:CZ	2:G:2:C:H2'	2.49	0.42
1:A:309:SER:O	1:A:313:GLU:HB3	2.19	0.42
1:B:172:LEU:HD11	1:B:472:TRP:CZ2	2.54	0.42
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.69	0.42
1:A:442:ARG:HE	1:C:397:GLU:HG2	1.84	0.42
1:D:316:TRP:O	1:D:319:SER:N	2.52	0.42
1:A:295:LEU:HD23	1:A:385:VAL:HG21	2.01	0.42
1:B:273:CYS:SG	1:B:274:VAL:N	2.93	0.42
1:F:327:SER:O	1:F:331:GLN:HG2	2.19	0.42
1:B:106:PHE:CE1	1:B:260:LEU:HD21	2.54	0.42
1:C:149:PRO:HB3	1:C:162:LEU:HB3	2.01	0.42
1:A:52:THR:HB	1:A:55:PHE:O	2.20	0.42
1:A:285:ILE:HG23	1:A:393:HIS:HD2	1.84	0.42
1:B:356:LEU:N	1:B:357:PRO:HD2	2.35	0.42
1:E:438:PRO:O	1:E:442:ARG:HG3	2.19	0.42
1:A:157:VAL:HG21	1:A:474:TYR:CE2	2.55	0.42
1:E:295:LEU:HD23	1:E:385:VAL:HG21	2.01	0.42
1:F:46:ARG:O	1:F:49:GLN:N	2.51	0.42
1:C:427:GLU:CD	1:C:436:ARG:HH12	2.28	0.41
1:C:428:LEU:HD11	1:C:441:SER:HA	2.02	0.41
1:F:320:ARG:HD2	1:F:320:ARG:HA	1.43	0.41
1:B:46:ARG:O	1:B:49:GLN:HG2	2.19	0.41
1:C:24:THR:HG23	1:C:27:GLU:CD	2.46	0.41
1:D:161:ARG:HB3	1:D:163:ARG:HH12	1.85	0.41
1:D:393:HIS:CG	1:D:394:PRO:HD2	2.54	0.41
1:E:334:MET:HE2	1:E:334:MET:HB3	1.88	0.41
1:B:264:MET:HG3	1:B:265:GLU:N	2.35	0.41
1:B:461:LYS:HB2	1:B:461:LYS:HE3	1.57	0.41
1:A:169:LEU:O	1:A:173:ARG:HG3	2.21	0.41
1:B:211:LYS:O	1:B:257:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:LEU:HD23	1:E:471:LEU:HD12	2.03	0.41
1:E:192:LEU:HD12	1:E:196:LEU:HB2	2.02	0.41
1:A:31:ILE:O	1:A:34:SER:HB3	2.21	0.41
1:A:192:LEU:HD12	1:A:196:LEU:HB2	2.03	0.41
1:C:163:ARG:HA	1:C:163:ARG:HD3	1.91	0.41
1:D:157:VAL:HG21	1:D:474:TYR:CE2	2.55	0.41
1:F:273:CYS:HB2	1:F:382:TYR:HB3	2.02	0.41
1:F:304:LYS:C	1:F:306:SER:H	2.27	0.41
1:A:229:LEU:CD2	1:A:257:ARG:HD3	2.47	0.41
1:A:264:MET:HG3	1:A:265:GLU:N	2.36	0.41
1:B:216:ALA:HA	1:B:233:PRO:HB3	2.02	0.41
1:D:273:CYS:HB2	1:D:382:TYR:HB3	2.02	0.41
1:E:479:ARG:HD3	1:E:479:ARG:HA	1.91	0.41
1:A:270:ILE:HG21	1:A:341:LEU:HD21	2.02	0.41
1:B:243:ILE:HA	1:B:243:ILE:HD13	1.82	0.41
1:E:157:VAL:HG21	1:E:474:TYR:CE2	2.56	0.41
1:B:52:THR:HB	1:B:55:PHE:O	2.21	0.40
1:C:278:GLU:HA	1:C:333:PHE:CZ	2.56	0.40
1:F:52:THR:HG22	1:F:57:LEU:HG	2.02	0.40
1:A:334:MET:HE2	1:A:334:MET:HB3	1.93	0.40
1:B:38:ARG:CZ	2:H:2:C:H2'	2.50	0.40
1:D:73:VAL:HG22	1:D:271:SER:HB2	2.02	0.40
1:D:309:SER:O	1:D:313:GLU:HB3	2.21	0.40
1:D:327:SER:OG	1:D:330:ASP:HB2	2.22	0.40
1:E:52:THR:HG22	1:E:57:LEU:HG	2.03	0.40
1:C:334:MET:HE2	1:C:334:MET:HB3	1.96	0.40
1:D:14:ARG:HG3	1:D:19:PRO:HD2	2.02	0.40
1:F:24:THR:HG23	1:F:27:GLU:CD	2.46	0.40
1:D:127:PHE:HZ	1:F:442:ARG:CZ	2.35	0.40
1:D:169:LEU:HA	1:D:169:LEU:HD23	1.81	0.40
1:D:438:PRO:O	1:D:442:ARG:HG3	2.21	0.40

All (2) 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:D:164:ASP:O	1:F:8:LYS:NZ[3_644]	2.03	0.17
1:A:26:HIS:NE2	1:C:465:ASP:OD2[3_544]	2.15	0.05

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	493/505 (98%)	454 (92%)	32 (6%)	7 (1%)	9	34
1	B	487/505 (96%)	453 (93%)	28 (6%)	6 (1%)	10	37
1	C	494/505 (98%)	468 (95%)	20 (4%)	6 (1%)	10	37
1	D	497/505 (98%)	465 (94%)	24 (5%)	8 (2%)	7	30
1	E	490/505 (97%)	466 (95%)	19 (4%)	5 (1%)	12	41
1	F	491/505 (97%)	462 (94%)	21 (4%)	8 (2%)	7	30
All	All	2952/3030 (97%)	2768 (94%)	144 (5%)	40 (1%)	9	34

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	304	LYS
1	B	301	GLN
1	D	326	ARG
1	F	301	GLN
1	A	310	LEU
1	A	311	VAL
1	B	310	LEU
1	B	311	VAL
1	C	272	TYR
1	C	304	LYS
1	C	310	LEU
1	D	272	TYR
1	D	325	SER
1	E	272	TYR
1	E	301	GLN
1	E	311	VAL
1	F	272	TYR
1	A	146	GLU
1	A	210	LEU

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Mol	Chain	Res	Type
1	B	210	LEU
1	B	302	HIS
1	C	311	VAL
1	D	310	LEU
1	D	311	VAL
1	E	310	LEU
1	F	149	PRO
1	F	306	SER
1	F	310	LEU
1	C	319	SER
1	D	210	LEU
1	F	300	GLY
1	F	304	LYS
1	F	311	VAL
1	A	61	ALA
1	C	210	LEU
1	D	301	GLN
1	B	299	TRP
1	E	210	LEU
1	D	270	ILE

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	430/450 (96%)	404 (94%)	26 (6%)	17	47
1	B	405/450 (90%)	386 (95%)	19 (5%)	23	55
1	C	432/450 (96%)	409 (95%)	23 (5%)	20	51
1	D	422/450 (94%)	400 (95%)	22 (5%)	21	51
1	E	431/450 (96%)	411 (95%)	20 (5%)	24	55
1	F	418/450 (93%)	397 (95%)	21 (5%)	22	53
All	All	2538/2700 (94%)	2407 (95%)	131 (5%)	21	51

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	57	LEU
1	A	63	VAL
1	A	68	THR
1	A	87	ARG
1	A	95	GLU
1	A	103	THR
1	A	119	ILE
1	A	143	GLU
1	A	147	SER
1	A	151	THR
1	A	167	GLU
1	A	193	VAL
1	A	198	ARG
1	A	264	MET
1	A	271	SER
1	A	272	TYR
1	A	286	PHE
1	A	318	LYS
1	A	328	THR
1	A	344	LEU
1	A	371	ASP
1	A	423	SER
1	A	436	ARG
1	A	479	ARG
1	A	485	ILE
1	B	3	GLN
1	B	24	THR
1	B	68	THR
1	B	103	THR
1	B	119	ILE
1	B	151	THR
1	B	152	ASP
1	B	193	VAL
1	B	198	ARG
1	B	264	MET
1	B	271	SER
1	B	272	TYR
1	B	286	PHE
1	B	302	HIS
1	B	344	LEU
1	B	371	ASP
1	B	423	SER

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Mol	Chain	Res	Type
1	B	479	ARG
1	B	485	ILE
1	C	24	THR
1	C	63	VAL
1	C	86	SER
1	C	87	ARG
1	C	92	LYS
1	C	103	THR
1	C	119	ILE
1	C	146	GLU
1	C	148	GLN
1	C	164	ASP
1	C	193	VAL
1	C	238	SER
1	C	264	MET
1	C	273	CYS
1	C	330	ASP
1	C	344	LEU
1	C	370	GLU
1	C	371	ASP
1	C	423	SER
1	C	479	ARG
1	C	485	ILE
1	C	495	ASP
1	C	503	VAL
1	D	24	THR
1	D	68	THR
1	D	86	SER
1	D	95	GLU
1	D	103	THR
1	D	119	ILE
1	D	139	ARG
1	D	150	LEU
1	D	164	ASP
1	D	193	VAL
1	D	238	SER
1	D	264	MET
1	D	273	CYS
1	D	302	HIS
1	D	329	GLU
1	D	330	ASP
1	D	344	LEU

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Mol	Chain	Res	Type
1	D	423	SER
1	D	436	ARG
1	D	479	ARG
1	D	485	ILE
1	D	495	ASP
1	E	24	THR
1	E	68	THR
1	E	86	SER
1	E	90	GLU
1	E	103	THR
1	E	119	ILE
1	E	167	GLU
1	E	193	VAL
1	E	238	SER
1	E	264	MET
1	E	273	CYS
1	E	318	LYS
1	E	330	ASP
1	E	344	LEU
1	E	370	GLU
1	E	371	ASP
1	E	423	SER
1	E	479	ARG
1	E	485	ILE
1	E	495	ASP
1	F	24	THR
1	F	68	THR
1	F	86	SER
1	F	103	THR
1	F	119	ILE
1	F	147	SER
1	F	193	VAL
1	F	238	SER
1	F	264	MET
1	F	273	CYS
1	F	284	ARG
1	F	320	ARG
1	F	327	SER
1	F	330	ASP
1	F	344	LEU
1	F	370	GLU
1	F	371	ASP

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Mol	Chain	Res	Type
1	F	423	SER
1	F	479	ARG
1	F	485	ILE
1	F	495	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	20	GLN
1	A	290	GLN
1	A	302	HIS
1	A	384	ASN
1	A	451	HIS
1	B	13	HIS
1	B	20	GLN
1	B	50	GLN
1	B	121	ASN
1	B	302	HIS
1	B	384	ASN
1	B	393	HIS
1	C	13	HIS
1	C	20	GLN
1	C	49	GLN
1	C	53	GLN
1	C	141	HIS
1	C	182	HIS
1	C	331	GLN
1	C	384	ASN
1	C	393	HIS
1	C	505	GLN
1	D	13	HIS
1	D	20	GLN
1	D	50	GLN
1	D	53	GLN
1	D	141	HIS
1	D	178	GLN
1	D	182	HIS
1	D	227	HIS
1	D	296	HIS
1	D	384	ASN
1	D	393	HIS

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Mol	Chain	Res	Type
1	E	13	HIS
1	E	20	GLN
1	E	49	GLN
1	E	50	GLN
1	E	53	GLN
1	E	141	HIS
1	E	182	HIS
1	E	194	HIS
1	E	302	HIS
1	E	331	GLN
1	E	384	ASN
1	E	393	HIS
1	E	505	GLN
1	F	13	HIS
1	F	20	GLN
1	F	50	GLN
1	F	53	GLN
1	F	141	HIS
1	F	182	HIS
1	F	194	HIS
1	F	227	HIS
1	F	331	GLN
1	F	384	ASN
1	F	393	HIS
1	F	445	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	0/3	-	-
2	H	0/3	-	-
All	All	0/6	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	499/505 (98%)	-0.43	1 (0%) 91 83	61, 104, 156, 212	0
1	B	495/505 (98%)	-0.25	2 (0%) 88 76	73, 125, 176, 213	0
1	C	500/505 (99%)	-0.43	4 (0%) 82 65	55, 89, 140, 204	0
1	D	501/505 (99%)	-0.34	4 (0%) 82 65	59, 113, 180, 217	0
1	E	496/505 (98%)	-0.49	2 (0%) 88 76	56, 84, 139, 193	0
1	F	497/505 (98%)	-0.33	1 (0%) 91 83	65, 110, 175, 219	0
2	G	3/3 (100%)	-0.32	0 100 100	95, 95, 109, 155	0
2	H	3/3 (100%)	0.65	1 (33%) 1 0	117, 117, 119, 204	0
All	All	2994/3036 (98%)	-0.38	15 (0%) 87 73	55, 104, 166, 219	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	ALA	4.4
1	C	273	CYS	4.0
1	D	58	GLU	3.9
1	D	273	CYS	3.5
1	C	59	ARG	3.4
1	C	62	ALA	3.0
2	H	1	C	2.5
1	A	57	LEU	2.4
1	E	273	CYS	2.4
1	B	56	PRO	2.2
1	D	29	LEU	2.1
1	C	2	ALA	2.1
1	F	58	GLU	2.1
1	B	148	GLN	2.1
1	E	127	PHE	2.1

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	MG	B	1000	1/1	0.72	0.10	134,134,134,134	0
3	MG	A	1000	1/1	0.91	0.06	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.