



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:51 PM UTC

PDB ID : 9PEP / pdb_00009pep
Title : Crystal structure of holo-pvspha
Authors : Hai, Y.; He, X.
Deposited on : 2025-07-02
Resolution : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

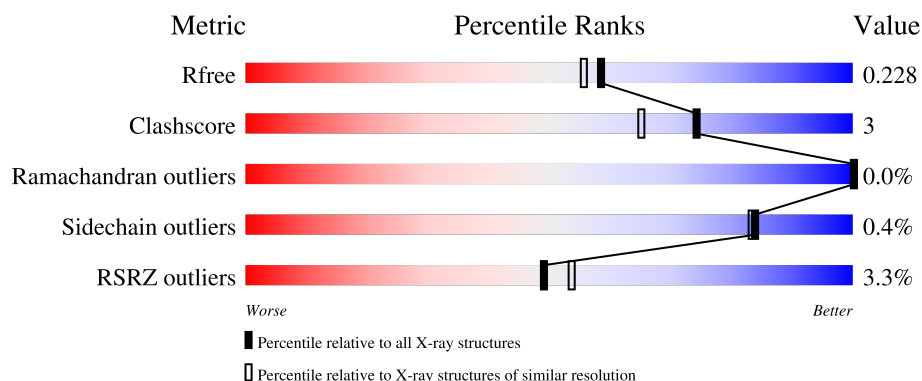
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	490	<div> <div>2%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>
1	B	490	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>6%</div> </div>
1	C	490	<div> <div>3%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	D	490	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	E	490	<div> <div>3%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	490	<div><div></div><div>2%</div><div>89%</div><div>• 7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22629 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 Aminoacyl transferase sphA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	P	S	0	0	0
			3556	2257	603	675	1	20			
1	B	462	Total	C	N	O	P	S	0	0	0
			3603	2286	611	684	1	21			
1	C	456	Total	C	N	O	P	S	0	0	0
			3555	2257	602	675	1	20			
1	D	456	Total	C	N	O	P	S	0	1	0
			3569	2265	608	674	1	21			
1	E	453	Total	C	N	O	P	S	0	0	0
			3538	2247	599	671	1	20			
1	F	454	Total	C	N	O	P	S	0	0	0
			3535	2246	597	671	1	20			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A443I7W9
A	-18	GLY	-	expression tag	UNP A0A443I7W9
A	-17	SER	-	expression tag	UNP A0A443I7W9
A	-16	SER	-	expression tag	UNP A0A443I7W9
A	-15	HIS	-	expression tag	UNP A0A443I7W9
A	-14	HIS	-	expression tag	UNP A0A443I7W9
A	-13	HIS	-	expression tag	UNP A0A443I7W9
A	-12	HIS	-	expression tag	UNP A0A443I7W9
A	-11	HIS	-	expression tag	UNP A0A443I7W9
A	-10	HIS	-	expression tag	UNP A0A443I7W9
A	-9	SER	-	expression tag	UNP A0A443I7W9
A	-8	SER	-	expression tag	UNP A0A443I7W9
A	-7	GLY	-	expression tag	UNP A0A443I7W9
A	-6	LEU	-	expression tag	UNP A0A443I7W9
A	-5	VAL	-	expression tag	UNP A0A443I7W9
A	-4	PRO	-	expression tag	UNP A0A443I7W9
A	-3	ARG	-	expression tag	UNP A0A443I7W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A443I7W9
A	-1	SER	-	expression tag	UNP A0A443I7W9
A	0	HIS	-	expression tag	UNP A0A443I7W9
B	-19	MET	-	initiating methionine	UNP A0A443I7W9
B	-18	GLY	-	expression tag	UNP A0A443I7W9
B	-17	SER	-	expression tag	UNP A0A443I7W9
B	-16	SER	-	expression tag	UNP A0A443I7W9
B	-15	HIS	-	expression tag	UNP A0A443I7W9
B	-14	HIS	-	expression tag	UNP A0A443I7W9
B	-13	HIS	-	expression tag	UNP A0A443I7W9
B	-12	HIS	-	expression tag	UNP A0A443I7W9
B	-11	HIS	-	expression tag	UNP A0A443I7W9
B	-10	HIS	-	expression tag	UNP A0A443I7W9
B	-9	SER	-	expression tag	UNP A0A443I7W9
B	-8	SER	-	expression tag	UNP A0A443I7W9
B	-7	GLY	-	expression tag	UNP A0A443I7W9
B	-6	LEU	-	expression tag	UNP A0A443I7W9
B	-5	VAL	-	expression tag	UNP A0A443I7W9
B	-4	PRO	-	expression tag	UNP A0A443I7W9
B	-3	ARG	-	expression tag	UNP A0A443I7W9
B	-2	GLY	-	expression tag	UNP A0A443I7W9
B	-1	SER	-	expression tag	UNP A0A443I7W9
B	0	HIS	-	expression tag	UNP A0A443I7W9
C	-19	MET	-	initiating methionine	UNP A0A443I7W9
C	-18	GLY	-	expression tag	UNP A0A443I7W9
C	-17	SER	-	expression tag	UNP A0A443I7W9
C	-16	SER	-	expression tag	UNP A0A443I7W9
C	-15	HIS	-	expression tag	UNP A0A443I7W9
C	-14	HIS	-	expression tag	UNP A0A443I7W9
C	-13	HIS	-	expression tag	UNP A0A443I7W9
C	-12	HIS	-	expression tag	UNP A0A443I7W9
C	-11	HIS	-	expression tag	UNP A0A443I7W9
C	-10	HIS	-	expression tag	UNP A0A443I7W9
C	-9	SER	-	expression tag	UNP A0A443I7W9
C	-8	SER	-	expression tag	UNP A0A443I7W9
C	-7	GLY	-	expression tag	UNP A0A443I7W9
C	-6	LEU	-	expression tag	UNP A0A443I7W9
C	-5	VAL	-	expression tag	UNP A0A443I7W9
C	-4	PRO	-	expression tag	UNP A0A443I7W9
C	-3	ARG	-	expression tag	UNP A0A443I7W9
C	-2	GLY	-	expression tag	UNP A0A443I7W9
C	-1	SER	-	expression tag	UNP A0A443I7W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A443I7W9
D	-19	MET	-	initiating methionine	UNP A0A443I7W9
D	-18	GLY	-	expression tag	UNP A0A443I7W9
D	-17	SER	-	expression tag	UNP A0A443I7W9
D	-16	SER	-	expression tag	UNP A0A443I7W9
D	-15	HIS	-	expression tag	UNP A0A443I7W9
D	-14	HIS	-	expression tag	UNP A0A443I7W9
D	-13	HIS	-	expression tag	UNP A0A443I7W9
D	-12	HIS	-	expression tag	UNP A0A443I7W9
D	-11	HIS	-	expression tag	UNP A0A443I7W9
D	-10	HIS	-	expression tag	UNP A0A443I7W9
D	-9	SER	-	expression tag	UNP A0A443I7W9
D	-8	SER	-	expression tag	UNP A0A443I7W9
D	-7	GLY	-	expression tag	UNP A0A443I7W9
D	-6	LEU	-	expression tag	UNP A0A443I7W9
D	-5	VAL	-	expression tag	UNP A0A443I7W9
D	-4	PRO	-	expression tag	UNP A0A443I7W9
D	-3	ARG	-	expression tag	UNP A0A443I7W9
D	-2	GLY	-	expression tag	UNP A0A443I7W9
D	-1	SER	-	expression tag	UNP A0A443I7W9
D	0	HIS	-	expression tag	UNP A0A443I7W9
E	-19	MET	-	initiating methionine	UNP A0A443I7W9
E	-18	GLY	-	expression tag	UNP A0A443I7W9
E	-17	SER	-	expression tag	UNP A0A443I7W9
E	-16	SER	-	expression tag	UNP A0A443I7W9
E	-15	HIS	-	expression tag	UNP A0A443I7W9
E	-14	HIS	-	expression tag	UNP A0A443I7W9
E	-13	HIS	-	expression tag	UNP A0A443I7W9
E	-12	HIS	-	expression tag	UNP A0A443I7W9
E	-11	HIS	-	expression tag	UNP A0A443I7W9
E	-10	HIS	-	expression tag	UNP A0A443I7W9
E	-9	SER	-	expression tag	UNP A0A443I7W9
E	-8	SER	-	expression tag	UNP A0A443I7W9
E	-7	GLY	-	expression tag	UNP A0A443I7W9
E	-6	LEU	-	expression tag	UNP A0A443I7W9
E	-5	VAL	-	expression tag	UNP A0A443I7W9
E	-4	PRO	-	expression tag	UNP A0A443I7W9
E	-3	ARG	-	expression tag	UNP A0A443I7W9
E	-2	GLY	-	expression tag	UNP A0A443I7W9
E	-1	SER	-	expression tag	UNP A0A443I7W9
E	0	HIS	-	expression tag	UNP A0A443I7W9
F	-19	MET	-	initiating methionine	UNP A0A443I7W9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP A0A443I7W9
F	-17	SER	-	expression tag	UNP A0A443I7W9
F	-16	SER	-	expression tag	UNP A0A443I7W9
F	-15	HIS	-	expression tag	UNP A0A443I7W9
F	-14	HIS	-	expression tag	UNP A0A443I7W9
F	-13	HIS	-	expression tag	UNP A0A443I7W9
F	-12	HIS	-	expression tag	UNP A0A443I7W9
F	-11	HIS	-	expression tag	UNP A0A443I7W9
F	-10	HIS	-	expression tag	UNP A0A443I7W9
F	-9	SER	-	expression tag	UNP A0A443I7W9
F	-8	SER	-	expression tag	UNP A0A443I7W9
F	-7	GLY	-	expression tag	UNP A0A443I7W9
F	-6	LEU	-	expression tag	UNP A0A443I7W9
F	-5	VAL	-	expression tag	UNP A0A443I7W9
F	-4	PRO	-	expression tag	UNP A0A443I7W9
F	-3	ARG	-	expression tag	UNP A0A443I7W9
F	-2	GLY	-	expression tag	UNP A0A443I7W9
F	-1	SER	-	expression tag	UNP A0A443I7W9
F	0	HIS	-	expression tag	UNP A0A443I7W9

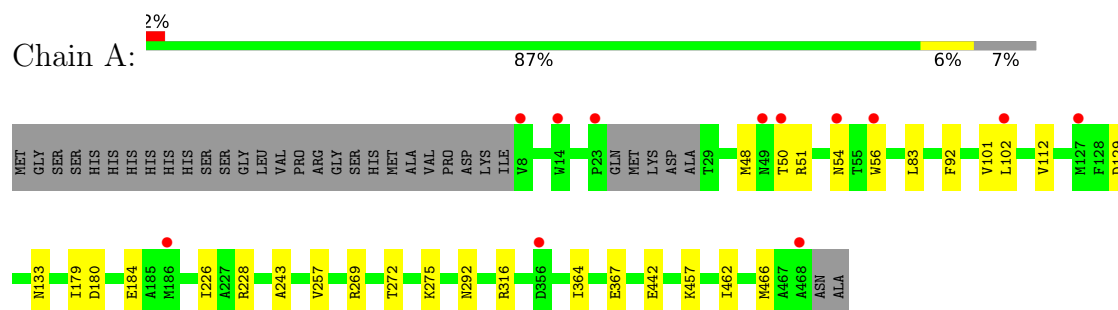
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	224	Total O 224 224	0	0
2	B	252	Total O 252 252	0	0
2	C	213	Total O 214 214	0	1
2	D	202	Total O 202 202	0	0
2	E	172	Total O 172 172	0	0
2	F	209	Total O 209 209	0	0

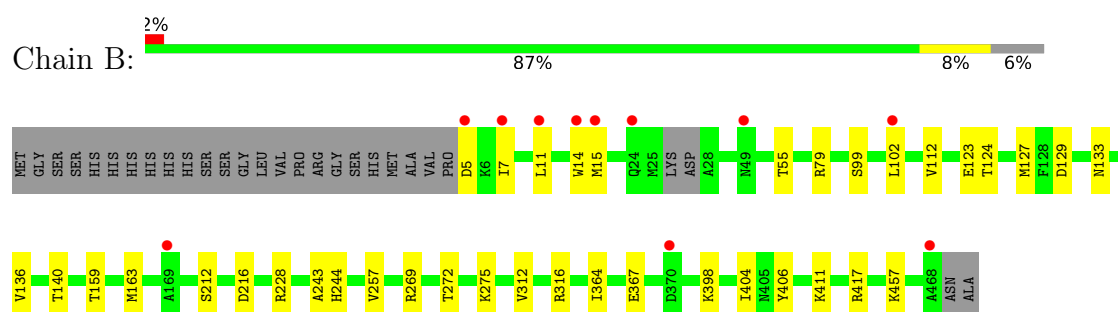
3 Residue-property plots [i](#)

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.

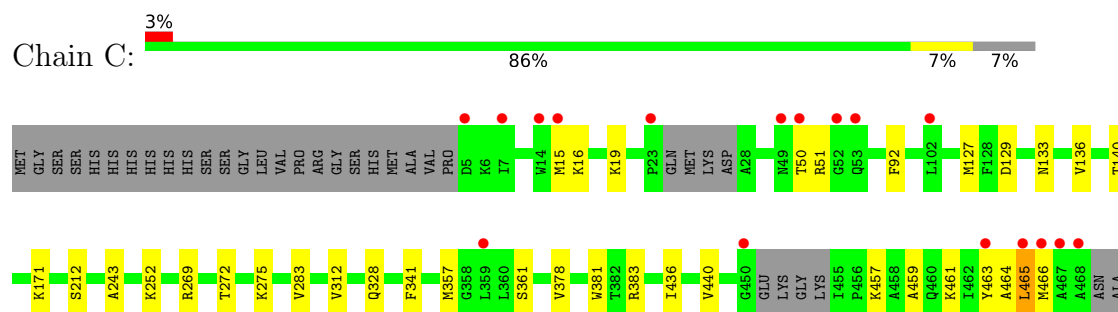
• Molecule 1: Aminoacyl transferase sphA



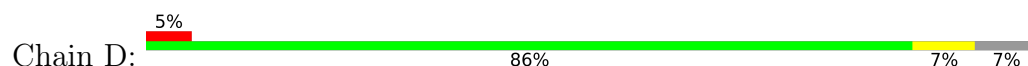
• Molecule 1: Aminoacyl transferase sphA

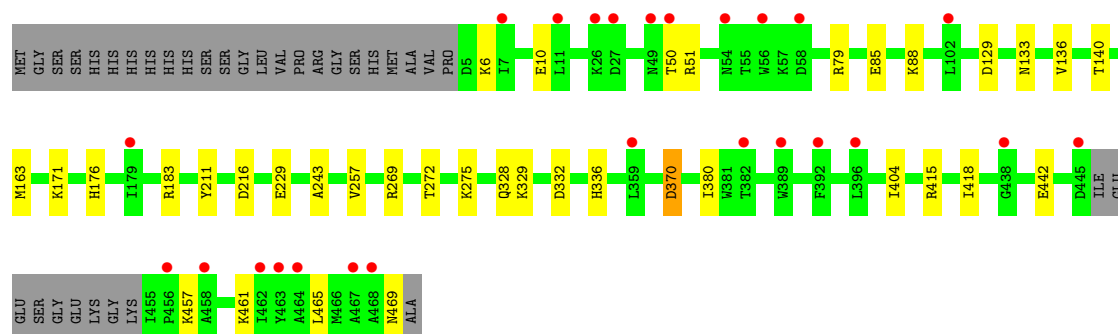


• Molecule 1: Aminoacyl transferase sphA

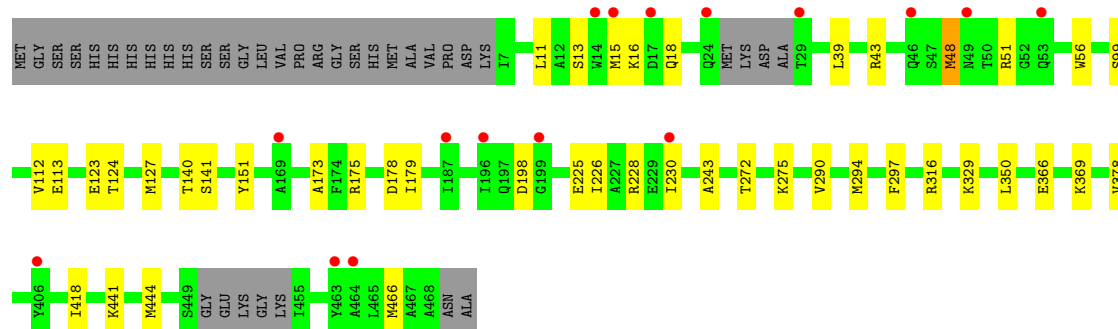
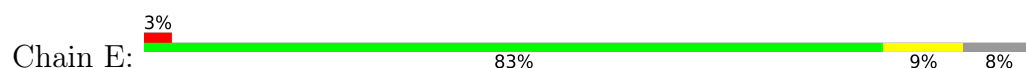


• Molecule 1: Aminoacyl transferase sphA

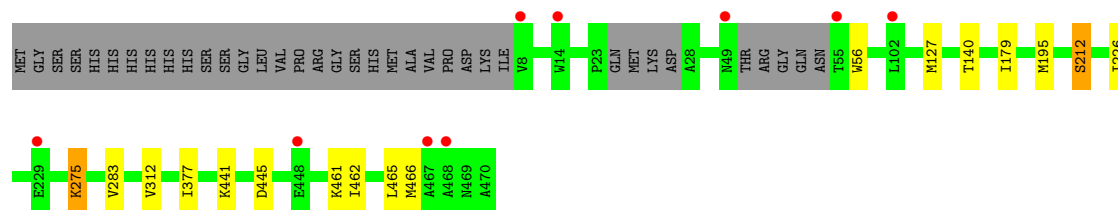
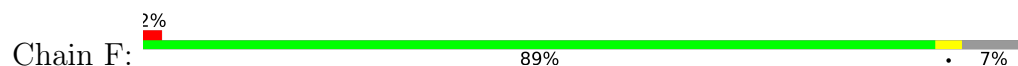




• Molecule 1: Aminoacyl transferase sphA



• Molecule 1: Aminoacyl transferase sphA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	242.96Å 101.63Å 172.00Å 90.00° 133.55° 90.00°	Depositor
Resolution (Å)	37.36 – 1.92 37.36 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.36-1.92) 98.1 (37.36-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.184 , 0.228 0.184 , 0.228	Depositor DCC
R_{free} test set	11447 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.004 for h,-k,-h-l 0.016 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22629	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0102e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.25	0/3601	0.44	0/4876
1	B	0.26	0/3648	0.43	0/4938
1	C	0.28	0/3599	0.45	0/4874
1	D	0.25	0/3617	0.42	0/4898
1	E	0.38	0/3582	0.54	0/4852
1	F	0.25	0/3579	0.42	0/4846
All	All	0.28	0/21626	0.45	0/29284

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3556	0	3534	22	0
1	B	3603	0	3584	26	0
1	C	3555	0	3531	22	0
1	D	3569	0	3554	26	0
1	E	3538	0	3514	35	0
1	F	3535	0	3512	11	0
2	A	224	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	252	0	0	3	0
2	C	214	0	0	2	0
2	D	202	0	0	3	0
2	E	172	0	0	3	0
2	F	209	0	0	2	0
All	All	22629	0	21229	133	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 3.

All (133) 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:18:GLN:HE22	1:E:48:MET:H	1.06	0.93
1:B:133:ASN:HD21	1:C:133:ASN:HD21	1.25	0.84
1:A:442:GLU:OE2	1:A:457:LYS:HD2	1.86	0.75
1:E:18:GLN:NE2	1:E:48:MET:H	1.85	0.73
1:E:18:GLN:HE22	1:E:48:MET:N	1.87	0.70
1:E:243:ALA:HA	1:E:272:THR:HG22	1.74	0.69
1:B:129:ASP:OD1	1:B:133:ASN:ND2	2.24	0.67
1:D:129:ASP:OD1	1:D:133:ASN:ND2	2.26	0.67
1:A:133:ASN:HD21	1:D:133:ASN:HD21	1.42	0.67
1:B:127:MET:HE1	1:B:312:VAL:HG22	1.77	0.66
1:B:269:ARG:HD2	2:B:515:HOH:O	1.96	0.65
1:B:228:ARG:NH2	2:B:502:HOH:O	2.30	0.65
1:C:269:ARG:HD2	2:C:504:HOH:O	1.97	0.63
1:D:370:ASP:OD1	1:D:370:ASP:N	2.31	0.63
1:D:465:LEU:O	1:D:469:ASN:ND2	2.31	0.63
1:B:123:GLU:HG2	1:B:124:THR:HG23	1.81	0.62
1:F:179:ILE:HG23	1:F:226:ILE:HD11	1.84	0.60
1:B:5:ASP:N	2:B:505:HOH:O	2.34	0.59
1:E:378:VAL:HB	1:E:418:ILE:HG12	1.82	0.59
1:A:54:ASN:HB3	1:A:56:TRP:CZ3	2.37	0.58
1:D:85:GLU:HA	1:D:88:LYS:HD3	1.85	0.58
1:B:243:ALA:HA	1:B:272:THR:HG22	1.84	0.58
1:B:257:VAL:HG11	1:B:269:ARG:HD3	1.84	0.58
1:E:112:VAL:HG22	1:E:316:ARG:HG3	1.84	0.58
1:E:123:GLU:HG2	1:E:124:THR:HG23	1.87	0.57
1:F:462:ILE:HG22	1:F:466:MET:HE3	1.85	0.57
1:C:127:MET:HE1	1:C:312:VAL:HG22	1.86	0.57
1:C:15:MET:HE3	1:C:466:MET:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASP:HB3	1:B:367:GLU:OE2	2.05	0.56
1:C:129:ASP:OD1	1:C:133:ASN:ND2	2.39	0.56
1:A:243:ALA:HA	1:A:272:THR:HG22	1.88	0.55
1:D:269:ARG:HD2	2:D:509:HOH:O	2.07	0.55
1:E:13:SER:HB3	1:E:51:ARG:NH2	2.21	0.55
1:A:269:ARG:HD2	2:A:513:HOH:O	2.05	0.55
1:B:7:ILE:HD13	1:B:398:LYS:HD3	1.89	0.55
1:D:6:LYS:O	1:D:10:GLU:HG2	2.07	0.55
1:E:13:SER:HA	1:E:16:LYS:NZ	2.23	0.54
1:A:228:ARG:NH2	2:A:502:HOH:O	2.34	0.54
1:C:459:ALA:O	1:C:463:TYR:HD1	1.90	0.54
1:A:292:ASN:OD1	1:D:50:THR:HG23	2.08	0.53
1:A:129:ASP:OD1	1:A:133:ASN:ND2	2.41	0.53
1:D:404:ILE:HB	1:D:415:ARG:HD2	1.91	0.53
1:E:441:LYS:HA	1:E:444:MET:HE3	1.90	0.53
1:B:406:TYR:CG	1:B:411:LYS:HD3	2.45	0.52
1:E:366:GLU:HG2	2:E:516:HOH:O	2.10	0.52
1:C:243:ALA:HA	1:C:272:THR:HG22	1.90	0.52
1:E:11:LEU:O	1:E:15:MET:HG3	2.10	0.51
1:C:136:VAL:O	1:C:140:THR:HG23	2.11	0.51
1:E:378:VAL:HB	1:E:418:ILE:CG1	2.41	0.51
1:B:133:ASN:ND2	1:C:133:ASN:HD21	2.02	0.50
1:C:140:THR:HG21	2:C:706:HOH:O	2.11	0.50
1:F:56:TRP:H	1:F:56:TRP:CD1	2.28	0.50
1:D:257:VAL:HG11	1:D:269:ARG:HD3	1.95	0.49
1:D:328:GLN:NE2	1:D:332:ASP:OD1	2.46	0.49
1:E:141:SER:HB2	1:E:297:PHE:HB2	1.94	0.48
1:D:163:MET:HB3	1:D:171:LYS:HD3	1.95	0.48
1:A:48:MET:HE3	1:A:50:THR:OG1	2.14	0.48
1:B:14:TRP:CE3	1:B:15:MET:HG3	2.49	0.48
1:A:50:THR:HG22	1:A:51:ARG:N	2.28	0.48
1:B:133:ASN:HD21	1:C:133:ASN:ND2	2.03	0.48
1:D:442:GLU:OE2	1:D:457:LYS:N	2.25	0.48
1:F:140:THR:HG21	2:F:704:HOH:O	2.14	0.47
1:A:180:ASP:O	1:A:184:GLU:HG2	2.15	0.47
1:A:462:ILE:O	1:A:466:MET:HG3	2.14	0.47
1:F:441:LYS:HE2	1:F:445:ASP:OD1	2.13	0.47
1:D:216:ASP:OD1	1:D:216:ASP:N	2.46	0.47
1:F:127:MET:HE1	1:F:312:VAL:HG22	1.96	0.47
1:F:275:LLP:H4'1	2:F:643:HOH:O	2.13	0.47
1:D:136:VAL:O	1:D:140:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:SER:HB3	1:C:381:TRP:HB2	1.97	0.46
1:E:228:ARG:NH2	2:E:509:HOH:O	2.49	0.46
1:E:56:TRP:CD1	1:E:56:TRP:H	2.32	0.46
1:E:113:GLU:HG2	1:E:127:MET:HG3	1.98	0.46
1:E:441:LYS:HA	1:E:444:MET:CE	2.46	0.46
1:F:127:MET:HG2	1:F:283:VAL:HG12	1.96	0.46
1:A:364:ILE:HA	1:A:367:GLU:HG2	1.98	0.46
1:B:212:SER:HB3	1:B:244:HIS:CD2	2.51	0.46
1:B:7:ILE:HG13	1:B:55:THR:HG21	1.98	0.46
1:A:101:VAL:O	1:A:102:LEU:HD23	2.16	0.45
1:C:465:LEU:HD22	1:C:465:LEU:HA	1.81	0.45
1:D:329:LYS:HE2	2:D:619:HOH:O	2.16	0.45
1:E:226:ILE:O	1:E:230:ILE:HG12	2.16	0.45
1:B:364:ILE:HA	1:B:367:GLU:HG2	1.98	0.45
1:E:39:LEU:HD22	1:E:48:MET:HE2	1.97	0.45
1:D:457:LYS:O	1:D:461:LYS:HD2	2.16	0.45
1:A:179:ILE:HG23	1:A:226:ILE:HD11	1.99	0.45
1:E:11:LEU:HA	1:E:11:LEU:HD23	1.80	0.45
1:C:357:MET:O	1:C:383:ARG:NH1	2.49	0.45
1:E:290:VAL:HG12	1:E:294:MET:HE2	1.98	0.45
1:D:243:ALA:HA	1:D:272:THR:HG22	2.00	0.44
1:A:257:VAL:HG11	1:A:269:ARG:HD3	1.99	0.44
1:E:175:ARG:HD3	1:E:178:ASP:OD2	2.18	0.44
1:E:418:ILE:O	1:E:418:ILE:HG13	2.16	0.44
1:E:140:THR:HG21	2:E:666:HOH:O	2.19	0.43
1:C:50:THR:HB	1:C:51:ARG:HH11	1.83	0.43
1:A:92:PHE:CZ	1:D:79:ARG:HG3	2.53	0.43
1:E:18:GLN:NE2	1:E:43:ARG:HA	2.34	0.42
1:A:133:ASN:ND2	1:D:133:ASN:HD21	2.12	0.42
1:E:18:GLN:HE21	1:E:43:ARG:HA	1.83	0.42
1:A:133:ASN:HD21	1:D:133:ASN:ND2	2.13	0.42
1:B:79:ARG:HG3	1:C:92:PHE:CZ	2.54	0.42
1:C:436:ILE:O	1:C:440:VAL:HG23	2.19	0.42
1:B:7:ILE:O	1:B:11:LEU:HD23	2.20	0.42
1:A:101:VAL:HG23	1:A:102:LEU:HG	2.02	0.42
1:B:112:VAL:HG22	1:B:316:ARG:HG3	2.01	0.42
1:E:366:GLU:O	1:E:369:LYS:HG2	2.20	0.42
1:B:159:THR:O	1:B:163:MET:HG3	2.20	0.41
1:E:151:TYR:CZ	1:E:173:ALA:HB2	2.55	0.41
1:F:212:SER:HA	1:F:377:ILE:HD13	2.02	0.41
1:C:252:LYS:HA	1:C:328:GLN:HE22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:SER:OG	1:B:102:LEU:HD12	2.20	0.41
1:C:457:LYS:O	1:C:461:LYS:HD3	2.20	0.41
1:D:176:HIS:HE1	1:D:211:TYR:CG	2.38	0.41
1:D:50:THR:HG22	1:D:51:ARG:HG3	2.03	0.41
1:A:112:VAL:HG22	1:A:316:ARG:HG3	2.02	0.41
1:E:13:SER:HB3	1:E:51:ARG:HH21	1.82	0.41
1:C:16:LYS:HA	1:C:19:LYS:NZ	2.35	0.41
1:E:350:LEU:HD13	1:E:444:MET:HE1	2.01	0.41
1:B:404:ILE:HG13	1:B:417:ARG:HG3	2.03	0.41
1:C:127:MET:HG2	1:C:283:VAL:HG12	2.03	0.41
1:D:183:ARG:NH2	1:D:229:GLU:OE1	2.54	0.41
1:E:466:MET:H	1:E:466:MET:HG2	1.64	0.41
1:F:195:MET:HE2	1:F:195:MET:HB3	1.89	0.41
1:F:461:LYS:O	1:F:465:LEU:HD13	2.20	0.41
1:E:179:ILE:HD12	1:E:179:ILE:HA	1.96	0.41
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.92	0.40
1:B:364:ILE:O	1:B:364:ILE:HG13	2.21	0.40
1:D:380:ILE:HG13	1:D:418:ILE:HD13	2.02	0.40
1:B:136:VAL:O	1:B:140:THR:HG23	2.21	0.40
1:C:341:PHE:HE2	1:C:378:VAL:HG11	1.85	0.40
1:E:13:SER:HA	1:E:16:LYS:HZ2	1.84	0.40
1:E:329:LYS:HB2	1:E:329:LYS:HE2	1.77	0.40
1:D:336:HIS:ND1	2:D:503:HOH:O	2.37	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	451/490 (92%)	443 (98%)	8 (2%)	0	100	100
1	B	457/490 (93%)	449 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	449/490 (92%)	441 (98%)	7 (2%)	1 (0%)	43	34
1	D	452/490 (92%)	442 (98%)	10 (2%)	0	100	100
1	E	446/490 (91%)	436 (98%)	10 (2%)	0	100	100
1	F	447/490 (91%)	440 (98%)	7 (2%)	0	100	100
All	All	2702/2940 (92%)	2651 (98%)	50 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	464	ALA

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	381/409 (93%)	381 (100%)	0	100	100
1	B	386/409 (94%)	385 (100%)	1 (0%)	86	86
1	C	381/409 (93%)	378 (99%)	3 (1%)	73	71
1	D	383/409 (94%)	382 (100%)	1 (0%)	86	86
1	E	380/409 (93%)	376 (99%)	4 (1%)	65	60
1	F	378/409 (92%)	377 (100%)	1 (0%)	86	86
All	All	2289/2454 (93%)	2279 (100%)	10 (0%)	84	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	457	LYS
1	C	171	LYS
1	C	212	SER
1	C	465	LEU
1	D	370	ASP
1	E	48	MET

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Mol	Chain	Res	Type
1	E	99	SER
1	E	198	ASP
1	E	225	GLU
1	F	212	SER

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	46	GLN
1	A	133	ASN
1	A	303	ASN
1	B	53	GLN
1	B	296	ASN
1	B	303	ASN
1	B	355	ASN
1	B	387	ASN
1	C	54	ASN
1	C	133	ASN
1	C	160	HIS
1	C	197	GLN
1	C	271	ASN
1	C	393	HIS
1	D	34	ASN
1	D	193	GLN
1	D	355	ASN
1	E	18	GLN
1	E	34	ASN
1	E	271	ASN
1	E	328	GLN
1	E	408	GLN
1	F	303	ASN
1	F	353	GLN
1	F	460	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	LLP	C	275	1	23,24,25	1.01	1 (4%)	25,32,34	1.32	3 (12%)
1	LLP	A	275	1	23,24,25	1.04	1 (4%)	25,32,34	1.45	5 (20%)
1	LLP	B	275	1	23,24,25	1.05	1 (4%)	25,32,34	1.46	4 (16%)
1	LLP	E	275	1	23,24,25	1.03	1 (4%)	25,32,34	1.38	3 (12%)
1	LLP	F	275	1	23,24,25	0.99	1 (4%)	25,32,34	1.29	2 (8%)
1	LLP	D	275	1	23,24,25	1.02	1 (4%)	25,32,34	1.30	2 (8%)

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
1	LLP	C	275	1	-	9/16/17/19	0/1/1/1
1	LLP	A	275	1	-	8/16/17/19	0/1/1/1
1	LLP	B	275	1	-	9/16/17/19	0/1/1/1
1	LLP	E	275	1	-	7/16/17/19	0/1/1/1
1	LLP	F	275	1	-	8/16/17/19	0/1/1/1
1	LLP	D	275	1	-	8/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	LLP	P-OP4	3.79	1.72	1.60
1	B	275	LLP	P-OP4	3.77	1.72	1.60
1	E	275	LLP	P-OP4	3.72	1.72	1.60
1	C	275	LLP	P-OP4	3.69	1.72	1.60
1	F	275	LLP	P-OP4	3.59	1.71	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	LLP	P-OP4	3.53	1.71	1.60

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	LLP	C4-C4'-NZ	-3.55	107.64	124.04
1	E	275	LLP	C4-C4'-NZ	-3.55	107.65	124.04
1	C	275	LLP	C4-C4'-NZ	-3.42	108.24	124.04
1	A	275	LLP	CE-NZ-C4'	3.41	129.63	118.72
1	D	275	LLP	C4-C4'-NZ	-3.39	108.41	124.04
1	C	275	LLP	CE-NZ-C4'	3.33	129.40	118.72
1	D	275	LLP	CE-NZ-C4'	3.18	128.92	118.72
1	F	275	LLP	CE-NZ-C4'	3.15	128.81	118.72
1	A	275	LLP	C4-C4'-NZ	-3.05	109.95	124.04
1	B	275	LLP	CE-NZ-C4'	3.05	128.50	118.72
1	E	275	LLP	CE-NZ-C4'	3.01	128.37	118.72
1	F	275	LLP	C4-C4'-NZ	-2.93	110.54	124.04
1	C	275	LLP	OP3-P-OP2	2.17	115.93	107.80
1	B	275	LLP	C3-C4-C4'	-2.08	116.64	120.40
1	B	275	LLP	C2'-C2-C3	-2.04	118.42	120.80
1	A	275	LLP	C5-C4-C4'	2.02	124.59	121.47
1	E	275	LLP	C2'-C2-C3	-2.02	118.43	120.80
1	A	275	LLP	CD-CG-CB	2.01	121.19	113.62
1	A	275	LLP	OP3-P-OP2	2.01	115.32	107.80

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	275	LLP	C5-C4-C4'-NZ
1	A	275	LLP	C5'-OP4-P-OP1
1	A	275	LLP	C5'-OP4-P-OP3
1	A	275	LLP	O-C-CA-CB
1	A	275	LLP	CG-CD-CE-NZ
1	B	275	LLP	C5-C4-C4'-NZ
1	B	275	LLP	O-C-CA-CB
1	C	275	LLP	C5'-OP4-P-OP1
1	C	275	LLP	O-C-CA-CB
1	D	275	LLP	C5'-OP4-P-OP1
1	D	275	LLP	O-C-CA-CB
1	E	275	LLP	C5-C4-C4'-NZ
1	E	275	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	F	275	LLP	C5'-OP4-P-OP1
1	F	275	LLP	O-C-CA-CB
1	C	275	LLP	CG-CD-CE-NZ
1	D	275	LLP	CG-CD-CE-NZ
1	F	275	LLP	CG-CD-CE-NZ
1	C	275	LLP	C3-C4-C4'-NZ
1	D	275	LLP	C3-C4-C4'-NZ
1	F	275	LLP	C5-C4-C4'-NZ
1	A	275	LLP	C3-C4-C4'-NZ
1	B	275	LLP	C3-C4-C4'-NZ
1	E	275	LLP	C3-C4-C4'-NZ
1	B	275	LLP	CA-CB-CG-CD
1	E	275	LLP	CG-CD-CE-NZ
1	F	275	LLP	C3-C4-C4'-NZ
1	B	275	LLP	C5'-OP4-P-OP1
1	A	275	LLP	CA-CB-CG-CD
1	D	275	LLP	C5-C4-C4'-NZ
1	E	275	LLP	CA-CB-CG-CD
1	B	275	LLP	C5'-OP4-P-OP3
1	C	275	LLP	C5'-OP4-P-OP3
1	D	275	LLP	C5'-OP4-P-OP3
1	F	275	LLP	C5'-OP4-P-OP3
1	C	275	LLP	C5-C4-C4'-NZ
1	E	275	LLP	CD-CE-NZ-C4'
1	B	275	LLP	C-CA-CB-CG
1	D	275	LLP	C-CA-CB-CG
1	E	275	LLP	C-CA-CB-CG
1	F	275	LLP	C-CA-CB-CG
1	B	275	LLP	CG-CD-CE-NZ
1	B	275	LLP	CD-CE-NZ-C4'
1	C	275	LLP	CD-CE-NZ-C4'
1	D	275	LLP	CD-CE-NZ-C4'
1	A	275	LLP	C5'-OP4-P-OP2
1	C	275	LLP	C5'-OP4-P-OP2
1	C	275	LLP	C-CA-CB-CG
1	F	275	LLP	CD-CE-NZ-C4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	275	LLP	1	0

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	455/490 (92%)	0.05	12 (2%) 57 63	17, 28, 51, 66	0
1	B	461/490 (94%)	0.05	11 (2%) 59 66	17, 28, 48, 63	0
1	C	455/490 (92%)	0.14	17 (3%) 45 50	16, 28, 53, 66	0
1	D	455/490 (92%)	0.29	25 (5%) 30 35	15, 31, 51, 61	1 (0%)
1	E	452/490 (92%)	0.41	16 (3%) 47 52	20, 33, 57, 70	0
1	F	453/490 (92%)	0.06	9 (1%) 65 71	18, 29, 51, 64	0
All	All	2731/2940 (92%)	0.17	90 (3%) 49 54	15, 29, 53, 70	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	463	TYR	4.3
1	A	49	ASN	3.9
1	D	359	LEU	3.8
1	F	49	ASN	3.8
1	B	102	LEU	3.8
1	C	465	LEU	3.8
1	E	196	ILE	3.7
1	E	463	TYR	3.7
1	E	406	TYR	3.6
1	E	14	TRP	3.5
1	D	27	ASP	3.5
1	D	463	TYR	3.4
1	F	55	THR	3.4
1	D	389	TRP	3.4
1	A	102	LEU	3.3
1	D	456	PRO	3.3
1	B	7	ILE	3.3
1	C	53	GLN	3.3
1	E	29	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	467	ALA	3.1
1	E	199	GLY	3.1
1	B	169	ALA	3.1
1	D	11	LEU	3.1
1	D	102	LEU	3.1
1	E	53	GLN	3.0
1	A	127	MET	3.0
1	A	54	ASN	3.0
1	D	7	ILE	3.0
1	C	450	GLY	2.9
1	D	464	ALA	2.9
1	A	50	THR	2.9
1	C	14	TRP	2.9
1	D	468	ALA	2.8
1	F	467	ALA	2.8
1	C	466	MET	2.8
1	A	56	TRP	2.8
1	B	370	ASP	2.8
1	C	49	ASN	2.8
1	D	396	LEU	2.8
1	C	467	ALA	2.7
1	C	23	PRO	2.7
1	C	468	ALA	2.7
1	F	448	GLU	2.7
1	E	15	MET	2.7
1	C	359	LEU	2.6
1	D	458	ALA	2.6
1	D	49	ASN	2.6
1	C	52	GLY	2.6
1	A	23	PRO	2.6
1	E	169	ALA	2.6
1	E	464	ALA	2.6
1	D	50	THR	2.6
1	E	46	GLN	2.5
1	D	438	GLY	2.5
1	B	15	MET	2.5
1	F	8	VAL	2.5
1	D	392	PHE	2.5
1	B	24	GLN	2.5
1	F	468	ALA	2.5
1	A	186	MET	2.4
1	C	15	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	382	THR	2.4
1	E	49	ASN	2.4
1	D	54	ASN	2.3
1	B	11	LEU	2.3
1	E	230	ILE	2.3
1	A	8	VAL	2.3
1	C	50	THR	2.3
1	A	356	ASP	2.3
1	B	468	ALA	2.2
1	F	102	LEU	2.2
1	D	445	ASP	2.2
1	D	26	LYS	2.2
1	C	7	ILE	2.1
1	D	179	ILE	2.1
1	B	5	ASP	2.1
1	E	17	ASP	2.1
1	F	229	GLU	2.1
1	E	187	ILE	2.1
1	D	58	ASP	2.1
1	A	14	TRP	2.1
1	D	56	TRP	2.1
1	A	468	ALA	2.1
1	E	24	GLN	2.1
1	C	102	LEU	2.1
1	D	462	ILE	2.0
1	B	49	ASN	2.0
1	B	14	TRP	2.0
1	F	14	TRP	2.0
1	C	5	ASP	2.0

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

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
1	LLP	F	275	24/25	0.95	0.09	16,24,39,50	0
1	LLP	E	275	24/25	0.96	0.07	22,26,38,45	0
1	LLP	C	275	24/25	0.97	0.07	17,21,35,52	0
1	LLP	A	275	24/25	0.97	0.07	15,24,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	B	275	24/25	0.97	0.06	16,22,39,43	0
1	LLP	D	275	24/25	0.98	0.06	18,23,40,42	0

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 [i](#)

There are no such residues in this entry.