



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FR4
Title : Crystal structure of human serine/threonine-protein kinase 32A (YANK1)
Authors : Chaikuad, A.; Elkins, J.M.; Krojer, T.; Mahajan, P.; Goubin, S.; Szklarz, M.; Tumber, A.; Wang, J.; Savitsky, P.; Shrestha, B.; Daga, N.; Picaud, S.; Fedorov, O.; Allerston, C.K.; Latwiel, S.V.A.; Vollmar, M.; Canning, P.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2012-06-26
Resolution : 2.29 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

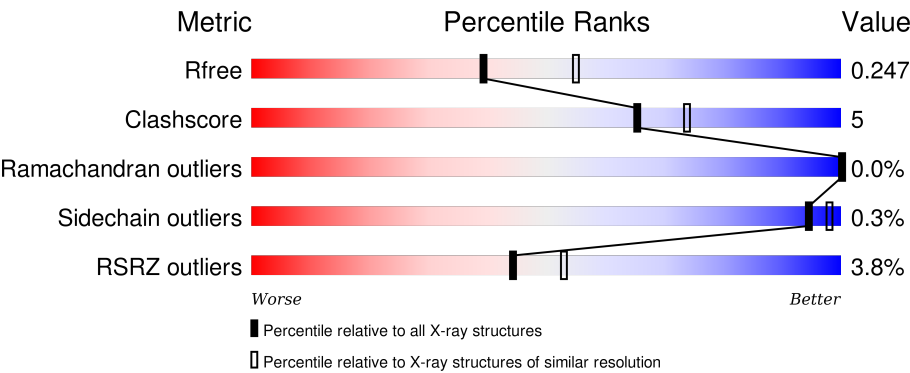
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	384	<div><div>2%</div><div>84%7%9%</div></div>
1	B	384	<div><div>4%</div><div>81%10%9%</div></div>
1	C	384	<div><div>2%</div><div>81%9%10%</div></div>
1	D	384	<div><div>4%</div><div>83%7%10%</div></div>
1	E	384	<div><div>4%</div><div>82%7%11%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	384	

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	EDO	B	402	-	-	-	X
3	EDO	B	403	-	-	-	X
3	EDO	C	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18277 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.

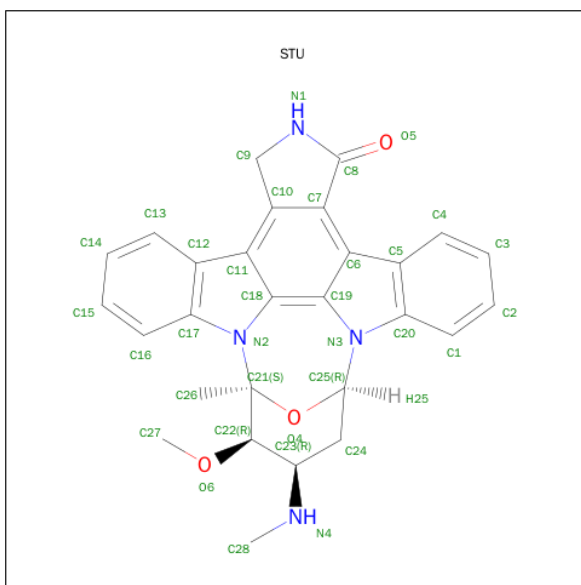
- Molecule 1 is a protein called Serine/threonine-protein kinase 32A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	7	0
			2871	1830	493	527	21			
1	B	350	Total	C	N	O	S	0	6	0
			2873	1831	490	531	21			
1	C	344	Total	C	N	O	S	0	6	0
			2833	1805	484	522	22			
1	D	346	Total	C	N	O	S	0	5	0
			2825	1806	477	521	21			
1	E	342	Total	C	N	O	S	0	6	0
			2810	1792	475	522	21			
1	F	346	Total	C	N	O	S	0	5	0
			2820	1800	478	522	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
A	0	MET	-	EXPRESSION TAG	UNP Q8WU08
B	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
B	0	MET	-	EXPRESSION TAG	UNP Q8WU08
C	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
C	0	MET	-	EXPRESSION TAG	UNP Q8WU08
D	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
D	0	MET	-	EXPRESSION TAG	UNP Q8WU08
E	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
E	0	MET	-	EXPRESSION TAG	UNP Q8WU08
F	-1	SER	-	EXPRESSION TAG	UNP Q8WU08
F	0	MET	-	EXPRESSION TAG	UNP Q8WU08

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		
2	C	1	Total	C	N	O	0	0
			35	28	4	3		
2	D	1	Total	C	N	O	0	0
			35	28	4	3		
2	E	1	Total	C	N	O	0	0
			35	28	4	3		
2	F	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	B	167	Total O 167 167	0	0
4	C	172	Total O 172 172	0	0
4	D	144	Total O 144 144	0	0

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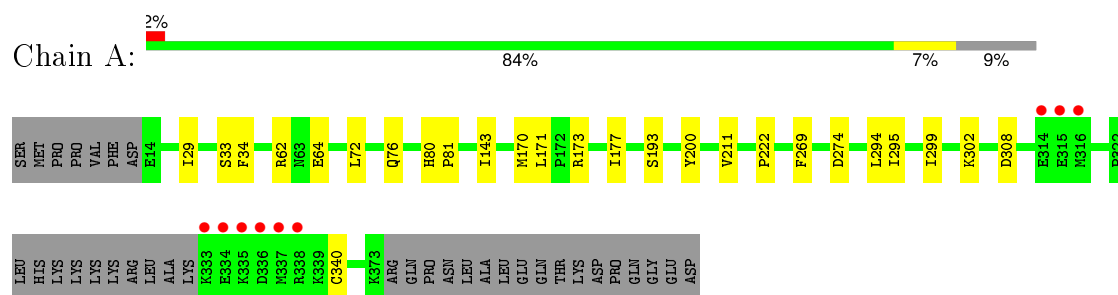
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	163	Total 163	O 163	0	0
4	F	173	Total 173	O 173	0	0

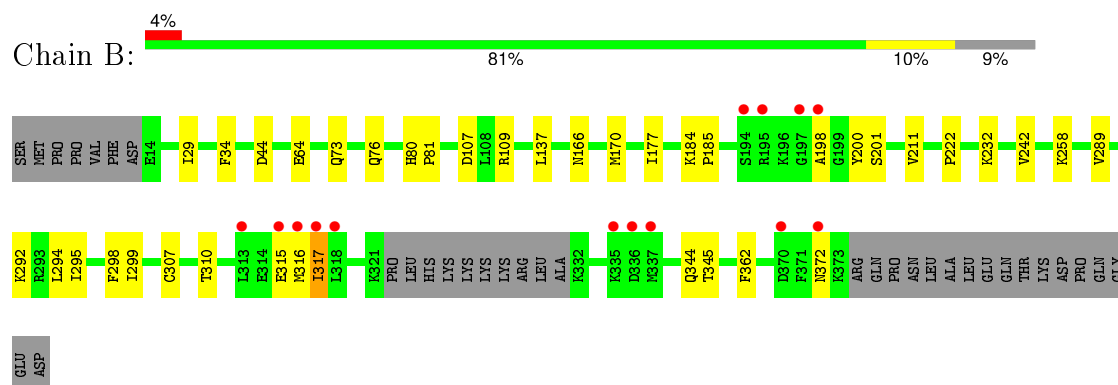
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

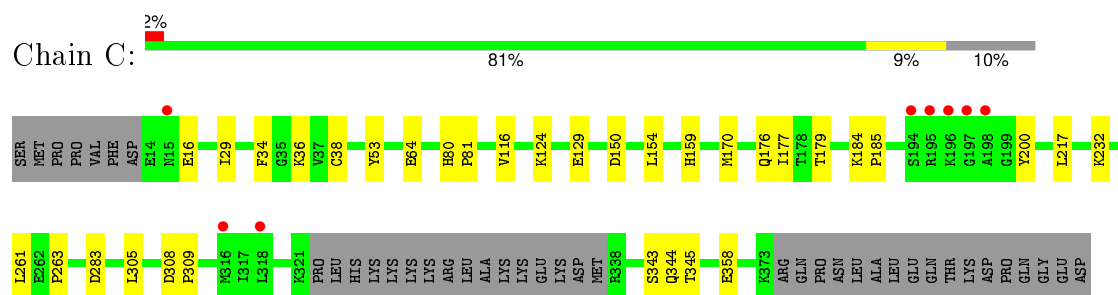
- Molecule 1: Serine/threonine-protein kinase 32A



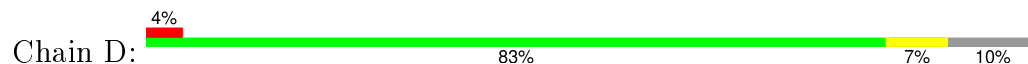
- Molecule 1: Serine/threonine-protein kinase 32A

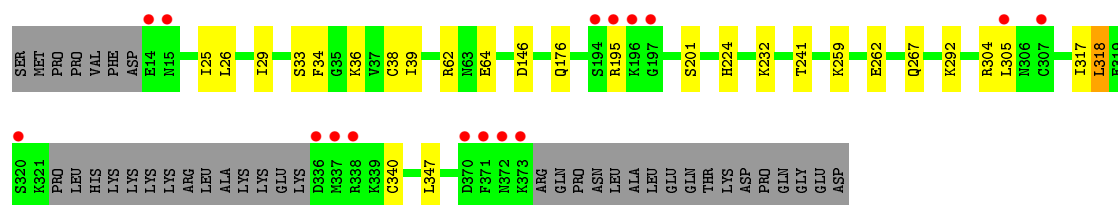


- Molecule 1: Serine/threonine-protein kinase 32A

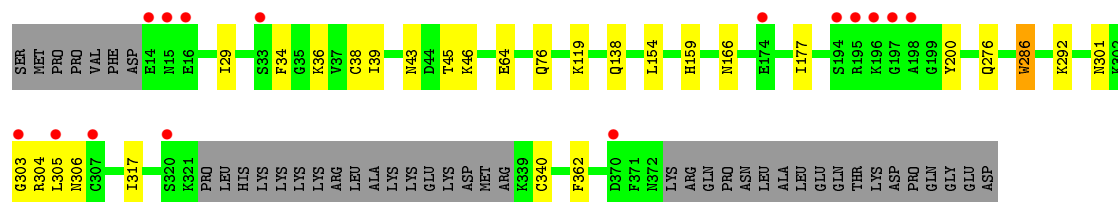
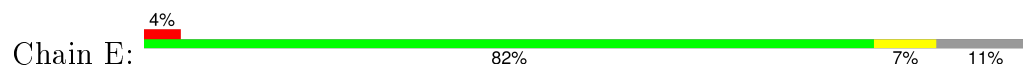


- Molecule 1: Serine/threonine-protein kinase 32A

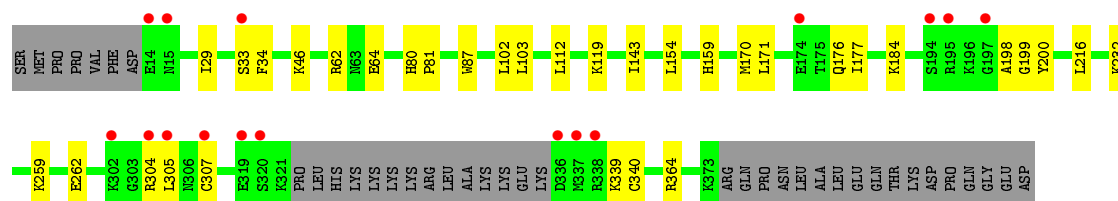
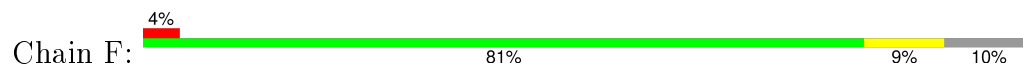




- Molecule 1: Serine/threonine-protein kinase 32A



- Molecule 1: Serine/threonine-protein kinase 32A



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	154.11Å 154.11Å 112.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.44 – 2.29 50.44 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.44-2.29) 95.7 (50.44-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.244 0.207 , 0.247	Depositor DCC
R_{free} test set	6741 reflections (5.53%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.3	EDS
Estimated twinning fraction	0.026 for -h,-k,l 0.000 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 128335 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18277	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 26.77 % 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 2.4797e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: STU, EDO

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	0.80	0/2958	0.58	0/3997
1	B	0.79	0/2956	0.56	0/3992
1	C	0.78	0/2916	0.57	0/3939
1	D	0.71	0/2906	0.52	0/3928
1	E	0.76	1/2892 (0.0%)	0.55	0/3908
1	F	0.76	0/2900	0.56	0/3920
All	All	0.77	1/17528 (0.0%)	0.56	0/23684

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	286	TRP	CD2-CE2	6.33	1.49	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	315	GLU	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	2871	0	2779	20	0
1	B	2873	0	2777	38	0
1	C	2833	0	2749	30	0
1	D	2825	0	2724	27	0
1	E	2810	0	2720	21	0
1	F	2820	0	2715	28	0
2	A	35	0	26	5	0
2	B	35	0	26	4	0
2	C	35	0	26	4	0
2	D	35	0	26	5	0
2	E	35	0	26	4	0
2	F	35	0	26	3	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	12	0	18	0	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
4	A	184	0	0	7	0
4	B	167	0	0	7	0
4	C	172	0	0	9	0
4	D	144	0	0	7	0
4	E	163	0	0	7	0
4	F	173	0	0	7	0
All	All	18277	0	16668	170	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 5.

All (170) 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)
2:B:401:STU:H16	2:B:401:STU:H261	1.52	0.91
2:C:401:STU:H261	2:C:401:STU:H16	1.56	0.86
2:E:401:STU:H16	2:E:401:STU:H261	1.61	0.83
2:A:401:STU:H261	2:A:401:STU:H16	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:STU:H16	2:D:401:STU:H261	1.63	0.80
1:C:38[B]:CYS:HG	1:C:53:TYR:HE2	1.33	0.77
1:D:26:LEU:HD13	1:D:318:LEU:HD22	1.68	0.74
2:F:401:STU:H261	2:F:401:STU:H16	1.69	0.73
1:D:224[A]:HIS:ND1	4:D:639:HOH:O	2.22	0.72
1:C:232:LYS:NZ	4:C:617:HOH:O	2.27	0.68
1:B:289:VAL:HG22	1:B:294:LEU:HD12	1.77	0.65
1:C:150:ASP:O	2:C:401:STU:H272	1.97	0.65
1:B:34:PHE:CZ	1:B:64:GLU:HG3	2.32	0.65
1:E:34:PHE:CZ	1:E:64:GLU:HG3	2.32	0.63
1:C:34:PHE:CZ	1:C:64:GLU:HG3	2.34	0.63
1:B:307:CYS:SG	1:F:307:CYS:CB	2.87	0.62
1:B:292:LYS:HA	4:B:578:HOH:O	1.99	0.62
1:E:39:ILE:HD13	1:E:317:ILE:HG21	1.81	0.61
1:A:193[A]:SER:OG	4:A:658:HOH:O	2.16	0.61
4:A:638:HOH:O	1:F:232:LYS:HE2	2.00	0.61
1:E:43:ASN:HB2	4:E:545:HOH:O	1.99	0.61
1:A:34:PHE:CZ	1:A:64:GLU:HG3	2.36	0.60
1:D:34:PHE:CZ	1:D:64:GLU:HG3	2.36	0.60
1:F:34:PHE:CZ	1:F:64:GLU:HG3	2.38	0.59
1:B:73[A]:GLN:OE1	1:B:170:MET:HE1	2.02	0.59
1:A:64:GLU:OE2	4:A:677:HOH:O	2.16	0.58
1:B:198:ALA:HB1	4:B:643:HOH:O	2.03	0.57
1:B:232:LYS:HG2	4:B:650:HOH:O	2.05	0.56
1:A:170:MET:HG2	4:A:633:HOH:O	2.06	0.56
1:D:292:LYS:NZ	4:D:549:HOH:O	2.29	0.56
2:B:401:STU:H261	2:B:401:STU:C16	2.23	0.56
1:C:38[B]:CYS:SG	1:C:53:TYR:HE2	2.29	0.56
1:E:76:GLN:HG2	1:E:362:PHE:CG	2.41	0.55
1:B:298:PHE:O	1:B:299:ILE:HD13	2.07	0.55
1:F:170:MET:HG2	4:F:642:HOH:O	2.05	0.55
1:B:201:SER:HB3	4:B:577:HOH:O	2.06	0.54
1:E:304:ARG:O	1:E:305:LEU:CB	2.56	0.54
1:D:241:THR:HG21	4:D:641:HOH:O	2.07	0.54
1:D:26:LEU:CD1	1:D:318:LEU:HD22	2.38	0.54
1:B:211:VAL:HG13	1:B:222:PRO:HD2	1.91	0.53
1:F:304:ARG:O	1:F:305:LEU:CB	2.56	0.53
2:C:401:STU:C16	2:C:401:STU:H261	2.26	0.53
1:D:262[B]:GLU:HG2	1:D:267:GLN:HB2	1.89	0.53
1:D:304:ARG:O	1:D:305:LEU:CB	2.57	0.53
1:F:184:LYS:HE3	4:F:518:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:GLN:HG2	1:E:362:PHE:CD2	2.44	0.52
2:B:401:STU:C26	2:B:401:STU:C16	2.87	0.52
1:A:143:ILE:HD11	1:A:171:LEU:HD22	1.92	0.52
1:F:259:LYS:CE	4:F:635:HOH:O	2.58	0.51
1:C:343:SER:HB2	1:D:347:LEU:CD1	2.40	0.51
1:E:29:ILE:HD12	2:E:401:STU:C5	2.40	0.51
2:F:401:STU:C16	2:F:401:STU:H261	2.40	0.51
1:E:34:PHE:CZ	1:E:64:GLU:CG	2.95	0.50
1:A:299:ILE:HB	4:A:679:HOH:O	2.12	0.50
1:C:179:THR:HG23	4:C:618:HOH:O	2.12	0.50
1:C:184:LYS:HE3	4:C:599:HOH:O	2.10	0.50
1:B:44:ASP:HA	1:F:46:LYS:HG2	1.94	0.50
1:E:36:LYS:HD2	1:E:38[A]:CYS:SG	2.52	0.49
1:A:269:PHE:CD1	1:A:274:ASP:HB3	2.47	0.49
2:D:401:STU:H273	2:D:401:STU:C17	2.43	0.49
1:F:177:ILE:HG22	1:F:200:TYR:O	2.12	0.49
2:E:401:STU:H261	2:E:401:STU:C16	2.32	0.49
1:C:34:PHE:CZ	1:C:64:GLU:CG	2.95	0.49
1:B:316:MET:HE2	4:C:534:HOH:O	2.12	0.49
1:B:34:PHE:CZ	1:B:64:GLU:CG	2.95	0.49
1:B:166:ASN:ND2	4:B:633:HOH:O	2.21	0.49
1:B:258:LYS:NZ	4:B:653:HOH:O	2.43	0.49
1:A:302:LYS:HE3	1:A:308:ASP:OD2	2.12	0.48
1:B:372:ASN:ND2	1:D:195:ARG:HA	2.28	0.48
1:B:344:GLN:HG3	1:B:345:THR:N	2.29	0.48
1:E:36:LYS:HG2	4:E:572:HOH:O	2.13	0.48
1:A:34:PHE:CZ	1:A:64:GLU:CG	2.96	0.48
1:A:211:VAL:HG13	1:A:222:PRO:HD2	1.96	0.48
1:A:294:LEU:HD22	1:F:62:ARG:NH2	2.28	0.47
1:F:143:ILE:HD11	1:F:171:LEU:HD22	1.96	0.47
1:C:36:LYS:HD2	1:C:38[A]:CYS:SG	2.53	0.47
1:C:344:GLN:HG3	1:C:345:THR:N	2.29	0.47
1:C:176[B]:GLN:NE2	4:C:553:HOH:O	2.45	0.47
1:E:34:PHE:CE2	1:E:64:GLU:HG3	2.49	0.47
2:C:401:STU:C26	2:C:401:STU:C16	2.92	0.47
1:D:34:PHE:CZ	1:D:64:GLU:CG	2.98	0.47
1:A:295:ILE:N	1:A:295:ILE:HD13	2.29	0.47
1:B:73[A]:GLN:OE1	1:B:170:MET:CE	2.61	0.47
1:D:36:LYS:HD2	1:D:38[B]:CYS:SG	2.55	0.47
1:D:146:ASP:HA	4:D:527:HOH:O	2.14	0.47
1:C:116:VAL:HA	4:C:641:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:LEU:HA	1:F:159:HIS:O	2.15	0.46
1:F:80:HIS:CG	1:F:81:PRO:HD2	2.51	0.46
2:A:401:STU:C16	2:A:401:STU:C26	2.94	0.46
1:D:29:ILE:HD12	2:D:401:STU:C5	2.46	0.46
1:F:198:ALA:HB1	4:F:609:HOH:O	2.15	0.46
1:C:261:LEU:O	1:C:263:PRO:HD3	2.16	0.46
1:E:166:ASN:HB3	4:E:628:HOH:O	2.15	0.46
1:A:173:ARG:NE	4:A:631:HOH:O	2.48	0.45
1:C:34:PHE:CE2	1:C:64:GLU:HG3	2.50	0.45
1:B:177:ILE:HG22	1:B:200:TYR:O	2.16	0.45
1:B:34:PHE:CE2	1:B:64:GLU:HG3	2.51	0.45
1:B:242:VAL:O	1:B:242:VAL:HG23	2.16	0.45
1:A:72:LEU:O	1:A:76:GLN:HG3	2.17	0.45
1:E:301:ASN:OD1	1:E:303:GLY:N	2.49	0.45
1:B:76:GLN:HG2	1:B:362:PHE:CD2	2.52	0.45
1:C:343:SER:HB3	1:D:347:LEU:HD12	1.98	0.44
1:A:29:ILE:HD12	2:A:401:STU:C5	2.48	0.44
1:B:295:ILE:HD13	1:B:295:ILE:N	2.32	0.44
2:A:401:STU:H16	2:A:401:STU:C26	2.40	0.44
1:F:87:TRP:CE3	1:F:364:ARG:HB3	2.53	0.44
1:C:343:SER:CB	1:D:347:LEU:HD12	2.48	0.44
1:A:177:ILE:HG22	1:A:200:TYR:O	2.17	0.44
1:E:154:LEU:HA	1:E:159:HIS:O	2.18	0.44
1:A:80:HIS:CG	1:A:81:PRO:HD2	2.53	0.43
1:F:339:LYS:HD2	4:F:670:HOH:O	2.18	0.43
1:F:34:PHE:CZ	1:F:64:GLU:CG	3.01	0.43
1:B:44:ASP:HA	1:F:46:LYS:CG	2.48	0.43
1:C:217:LEU:HD22	4:C:591:HOH:O	2.17	0.43
1:B:289:VAL:CG2	1:B:294:LEU:HD12	2.45	0.43
1:A:34:PHE:CE2	1:A:64:GLU:HG3	2.54	0.43
1:A:299:ILE:HG21	4:A:683:HOH:O	2.19	0.43
1:D:232:LYS:HG2	4:D:612:HOH:O	2.19	0.43
1:B:242:VAL:O	1:B:242:VAL:CG2	2.67	0.43
2:D:401:STU:C26	2:D:401:STU:C16	2.96	0.42
1:D:34:PHE:CE2	1:D:64:GLU:HG3	2.54	0.42
1:E:306:ASN:N	4:E:517:HOH:O	2.52	0.42
1:C:232:LYS:HG2	4:C:550:HOH:O	2.20	0.42
1:D:39:ILE:HD13	1:D:317:ILE:HG21	2.01	0.42
1:E:45:THR:O	1:E:46:LYS:HB2	2.19	0.42
1:D:176:GLN:NE2	4:D:634:HOH:O	2.46	0.42
1:C:80:HIS:CG	1:C:81:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:HD22	1:D:62:ARG:NH2	2.35	0.42
2:A:401:STU:C17	2:A:401:STU:H273	2.50	0.42
1:F:29:ILE:HD12	2:F:401:STU:C5	2.49	0.42
1:B:317:ILE:HG22	1:C:170:MET:HB3	2.01	0.42
1:B:184:LYS:N	1:B:185:PRO:HD2	2.33	0.42
1:C:177:ILE:HG22	1:C:200:TYR:O	2.19	0.42
1:E:276:GLN:HG2	1:E:286:TRP:NE1	2.35	0.41
1:F:262:GLU:HB3	4:F:636:HOH:O	2.19	0.41
1:C:184:LYS:N	1:C:185:PRO:HD2	2.35	0.41
1:B:80:HIS:CG	1:B:81:PRO:HD2	2.55	0.41
1:F:102:LEU:C	1:F:103:LEU:HD22	2.39	0.41
1:F:119:LYS:HD3	4:F:662:HOH:O	2.20	0.41
1:F:176:GLN:CD	1:F:199:GLY:HA3	2.40	0.41
1:B:76:GLN:HG2	1:B:362:PHE:CG	2.56	0.41
1:A:33:SER:HB2	1:A:62:ARG:HH12	1.85	0.41
1:E:138:GLN:HB2	4:E:520:HOH:O	2.19	0.41
1:D:262[B]:GLU:HG2	1:D:267:GLN:CB	2.51	0.41
1:F:112:LEU:HD21	1:F:216:LEU:HA	2.03	0.41
1:C:129:GLU:OE2	1:C:159:HIS:ND1	2.43	0.41
1:D:201:SER:HB3	4:D:581:HOH:O	2.21	0.41
2:E:401:STU:C26	2:E:401:STU:C16	2.98	0.41
1:B:294:LEU:HD22	1:D:62:ARG:HH22	1.85	0.41
1:C:154:LEU:HA	1:C:159:HIS:O	2.21	0.41
1:E:177:ILE:HG22	1:E:200:TYR:O	2.21	0.41
1:E:119:LYS:HE3	4:E:650:HOH:O	2.20	0.41
1:D:25:ILE:HG23	1:D:38[A]:CYS:SG	2.61	0.40
1:D:259:LYS:HA	1:D:259:LYS:HD2	1.98	0.40
1:B:107:ASP:OD2	1:B:109:ARG:HB3	2.21	0.40
1:F:34:PHE:CE2	1:F:64:GLU:HG3	2.55	0.40
1:B:258:LYS:HE2	4:B:653:HOH:O	2.21	0.40
1:C:29:ILE:HG22	1:C:305:LEU:HD21	2.02	0.40
1:B:29:ILE:HD12	2:B:401:STU:C5	2.51	0.40
2:D:401:STU:H261	2:D:401:STU:C16	2.34	0.40
1:C:124:LYS:NZ	1:C:283:ASP:OD1	2.46	0.40
1:D:33:SER:HB2	1:D:62:ARG:HH12	1.86	0.40
1:F:33:SER:HB2	1:F:62:ARG:HH12	1.87	0.40
1:F:103:LEU:N	1:F:103:LEU:HD22	2.37	0.40
1:B:44:ASP:CB	1:F:46:LYS:HE2	2.52	0.40
1:B:137:LEU:HA	1:B:137:LEU:HD23	1.94	0.40
1:B:310:THR:HG22	1:C:358:GLU:CD	2.42	0.40
1:C:308:ASP:HA	1:C:309:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:LYS:HA	4:E:612:HOH:O	2.21	0.40
1:C:16:GLU:HA	4:C:567:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/384 (92%)	332 (94%)	21 (6%)	0	100	100
1	B	352/384 (92%)	334 (95%)	17 (5%)	1 (0%)	46	57
1	C	346/384 (90%)	326 (94%)	20 (6%)	0	100	100
1	D	347/384 (90%)	325 (94%)	22 (6%)	0	100	100
1	E	344/384 (90%)	324 (94%)	20 (6%)	0	100	100
1	F	347/384 (90%)	326 (94%)	21 (6%)	0	100	100
All	All	2089/2304 (91%)	1967 (94%)	121 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	ILE

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	315/355 (89%)	314 (100%)	1 (0%)	94	98
1	B	315/355 (89%)	315 (100%)	0	100	100
1	C	314/355 (88%)	314 (100%)	0	100	100
1	D	309/355 (87%)	307 (99%)	2 (1%)	90	96
1	E	311/355 (88%)	310 (100%)	1 (0%)	94	98
1	F	308/355 (87%)	307 (100%)	1 (0%)	94	98
All	All	1872/2130 (88%)	1867 (100%)	5 (0%)	94	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	CYS
1	D	318	LEU
1	D	340	CYS
1	E	340	CYS
1	F	340	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	STU	A	401	-	27,42,42	2.09	9 (33%)	23,68,68	1.63	4 (17%)
3	EDO	A	402	-	3,3,3	0.49	0	2,2,2	0.33	0
2	STU	B	401	-	27,42,42	2.20	9 (33%)	23,68,68	1.68	5 (21%)
3	EDO	B	402	-	3,3,3	0.89	0	2,2,2	0.45	0
3	EDO	B	403	-	3,3,3	0.82	0	2,2,2	0.20	0
2	STU	C	401	-	27,42,42	1.96	7 (25%)	23,68,68	1.66	5 (21%)
3	EDO	C	402	-	3,3,3	0.67	0	2,2,2	0.07	0
3	EDO	C	403	-	3,3,3	0.59	0	2,2,2	0.32	0
3	EDO	C	404	-	3,3,3	0.55	0	2,2,2	0.29	0
2	STU	D	401	-	27,42,42	2.20	6 (22%)	23,68,68	1.59	4 (17%)
2	STU	E	401	-	27,42,42	2.25	7 (25%)	23,68,68	1.62	4 (17%)
3	EDO	E	402	-	3,3,3	0.61	0	2,2,2	0.36	0
2	STU	F	401	-	27,42,42	2.11	8 (29%)	23,68,68	1.67	4 (17%)
3	EDO	F	402	-	3,3,3	0.57	0	2,2,2	0.28	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
2	STU	A	401	-	-	0/4/42/42	0/0/8/8
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
2	STU	B	401	-	-	0/4/42/42	0/0/8/8
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
2	STU	C	401	-	-	0/4/42/42	0/0/8/8
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
3	EDO	C	403	-	-	0/1/1/1	0/0/0/0
3	EDO	C	404	-	-	0/1/1/1	0/0/0/0
2	STU	D	401	-	-	0/4/42/42	0/0/8/8
2	STU	E	401	-	-	0/4/42/42	0/0/8/8
3	EDO	E	402	-	-	0/1/1/1	0/0/0/0
2	STU	F	401	-	-	0/4/42/42	0/0/8/8
3	EDO	F	402	-	-	0/1/1/1	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	STU	C22-C23	-4.81	1.48	1.52
2	B	401	STU	C22-C23	-3.95	1.48	1.52
2	C	401	STU	C22-C23	-3.28	1.49	1.52
2	F	401	STU	C22-C23	-3.13	1.49	1.52
2	A	401	STU	C22-C23	-2.96	1.49	1.52
2	B	401	STU	C13-C12	-2.58	1.35	1.41
2	C	401	STU	O5-C8	2.02	1.27	1.23
2	B	401	STU	C3-C4	2.04	1.41	1.36
2	A	401	STU	C7-C10	2.08	1.45	1.40
2	B	401	STU	C12-C17	2.14	1.44	1.41
2	A	401	STU	O5-C8	2.17	1.27	1.23
2	F	401	STU	C15-C16	2.24	1.41	1.36
2	F	401	STU	C26-C21	2.36	1.54	1.51
2	A	401	STU	C12-C17	2.61	1.45	1.41
2	B	401	STU	C19-C18	2.66	1.48	1.41
2	D	401	STU	O5-C8	2.68	1.28	1.23
2	A	401	STU	C26-C21	2.71	1.55	1.51
2	D	401	STU	C19-C18	2.74	1.48	1.41
2	A	401	STU	C19-C18	2.77	1.48	1.41
2	E	401	STU	O5-C8	2.81	1.29	1.23
2	C	401	STU	C5-C20	2.84	1.45	1.41
2	B	401	STU	O5-C8	2.85	1.29	1.23
2	A	401	STU	C7-C6	2.91	1.47	1.43
2	E	401	STU	C12-C17	3.05	1.46	1.41
2	F	401	STU	C19-C18	3.07	1.49	1.41
2	F	401	STU	C12-C17	3.08	1.46	1.41
2	C	401	STU	C19-C18	3.16	1.49	1.41
2	E	401	STU	C19-C18	3.27	1.49	1.41
2	F	401	STU	C5-C20	3.42	1.46	1.41
2	C	401	STU	C12-C17	3.45	1.47	1.41
2	D	401	STU	C12-C17	3.46	1.47	1.41
2	B	401	STU	C7-C6	3.52	1.48	1.43
2	F	401	STU	C7-C6	3.57	1.48	1.43
2	E	401	STU	C10-C11	3.60	1.48	1.42
2	C	401	STU	C7-C6	3.65	1.49	1.43
2	A	401	STU	C5-C20	4.14	1.48	1.41
2	B	401	STU	C5-C20	4.21	1.48	1.41
2	D	401	STU	C7-C6	4.40	1.50	1.43
2	E	401	STU	C5-C20	4.47	1.48	1.41
2	D	401	STU	C5-C20	4.54	1.48	1.41
2	C	401	STU	C10-C11	4.61	1.50	1.42
2	E	401	STU	C7-C6	4.72	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	STU	C10-C11	5.14	1.50	1.42
2	A	401	STU	C10-C11	5.42	1.51	1.42
2	B	401	STU	C10-C11	5.47	1.51	1.42
2	D	401	STU	C10-C11	5.70	1.51	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	STU	C24-C23-N4	-3.01	105.36	112.16
2	E	401	STU	C16-C17-C12	-2.59	117.00	120.73
2	C	401	STU	C16-C17-C12	-2.34	117.36	120.73
2	C	401	STU	C1-C20-C5	-2.24	117.50	120.73
2	D	401	STU	C3-C4-C5	-2.22	116.95	120.79
2	F	401	STU	C1-C20-C5	-2.21	117.54	120.73
2	A	401	STU	C1-C20-C5	-2.15	117.63	120.73
2	A	401	STU	C3-C4-C5	-2.12	117.12	120.79
2	B	401	STU	C16-C17-C12	-2.11	117.68	120.73
2	E	401	STU	O5-C8-C7	-2.03	125.23	128.62
2	B	401	STU	C4-C5-C20	2.09	122.03	119.39
2	D	401	STU	C13-C12-C17	2.39	122.41	119.39
2	F	401	STU	C13-C12-C17	2.42	122.46	119.39
2	E	401	STU	C13-C12-C17	2.46	122.51	119.39
2	C	401	STU	C4-C5-C20	2.58	122.66	119.39
2	C	401	STU	C13-C12-C17	2.58	122.66	119.39
2	D	401	STU	C4-C5-C20	2.60	122.68	119.39
2	F	401	STU	C4-C5-C20	2.97	123.15	119.39
2	B	401	STU	C13-C12-C17	3.05	123.25	119.39
2	A	401	STU	C4-C5-C20	3.11	123.32	119.39
2	A	401	STU	C16-C17-N2	4.24	137.40	132.22
2	D	401	STU	C16-C17-N2	4.53	137.76	132.22
2	B	401	STU	C16-C17-N2	4.62	137.87	132.22
2	E	401	STU	C16-C17-N2	4.65	137.90	132.22
2	F	401	STU	C16-C17-N2	4.73	138.00	132.22
2	C	401	STU	C16-C17-N2	4.94	138.25	132.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	STU	5	0
2	B	401	STU	4	0
2	C	401	STU	4	0
2	D	401	STU	5	0
2	E	401	STU	4	0
2	F	401	STU	3	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	350/384 (91%)	-0.37	9 (2%) 59 68	16, 36, 99, 134	0
1	B	350/384 (91%)	-0.25	14 (4%) 42 51	19, 37, 106, 148	0
1	C	344/384 (89%)	-0.30	8 (2%) 64 72	17, 37, 89, 131	0
1	D	346/384 (90%)	-0.17	16 (4%) 36 45	24, 47, 103, 128	0
1	E	342/384 (89%)	-0.16	15 (4%) 38 47	18, 42, 93, 124	0
1	F	346/384 (90%)	-0.24	16 (4%) 36 45	18, 40, 98, 136	0
All	All	2078/2304 (90%)	-0.25	78 (3%) 44 53	16, 40, 97, 148	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	MET	6.1
1	B	336	ASP	6.0
1	E	196	LYS	5.7
1	A	336	ASP	5.5
1	A	337	MET	5.3
1	D	305	LEU	4.8
1	B	195	ARG	4.8
1	F	336	ASP	4.7
1	E	15	ASN	4.6
1	D	15	ASN	4.5
1	E	194	SER	4.5
1	F	338	ARG	4.3
1	D	372	ASN	4.1
1	F	15	ASN	4.1
1	E	195	ARG	4.1
1	D	194	SER	4.0
1	F	337	MET	3.9
1	F	197	GLY	3.9
1	B	194	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	336	ASP	3.8
1	A	335	LYS	3.8
1	D	338	ARG	3.8
1	F	307	CYS	3.7
1	E	198	ALA	3.4
1	E	197	GLY	3.4
1	E	307	CYS	3.4
1	C	195	ARG	3.4
1	C	197	GLY	3.4
1	A	315	GLU	3.3
1	E	14	GLU	3.3
1	D	307	CYS	3.3
1	A	316	MET	3.2
1	C	196	LYS	3.2
1	B	335	LYS	3.2
1	A	333	LYS	3.1
1	B	315	GLU	3.0
1	B	370	ASP	2.8
1	F	194	SER	2.8
1	F	305	LEU	2.8
1	F	304	ARG	2.8
1	B	197	GLY	2.8
1	C	198	ALA	2.8
1	E	320	SER	2.8
1	F	33	SER	2.7
1	A	338	ARG	2.7
1	D	320	SER	2.6
1	E	16	GLU	2.6
1	E	370	ASP	2.6
1	D	197	GLY	2.5
1	B	317	ILE	2.5
1	D	370	ASP	2.5
1	F	320	SER	2.5
1	E	174	GLU	2.5
1	F	174	GLU	2.5
1	B	337	MET	2.4
1	D	195	ARG	2.4
1	A	334	GLU	2.4
1	C	194	SER	2.4
1	E	305	LEU	2.4
1	D	14	GLU	2.4
1	C	15	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	316	MET	2.3
1	B	198	ALA	2.3
1	F	14	GLU	2.3
1	B	316	MET	2.3
1	F	302	LYS	2.2
1	B	372	ASN	2.2
1	F	195	ARG	2.2
1	B	318	LEU	2.2
1	E	303	GLY	2.2
1	D	371	PHE	2.2
1	D	196	LYS	2.1
1	B	313	LEU	2.1
1	C	318	LEU	2.1
1	D	373	LYS	2.1
1	F	319	GLU	2.0
1	E	33	SER	2.0
1	A	314	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	B	402	4/4	0.78	0.18	6.43	40,42,42,48	0
3	EDO	C	402	4/4	0.92	0.39	5.40	55,56,58,60	0
3	EDO	B	403	4/4	0.99	0.14	2.71	29,30,35,36	0
3	EDO	C	403	4/4	0.95	0.14	1.41	37,40,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	E	402	4/4	0.91	0.14	1.22	42,50,52,53	0
3	EDO	A	402	4/4	0.87	0.22	1.03	55,55,56,56	0
2	STU	D	401	35/35	0.97	0.11	0.69	25,35,40,42	0
2	STU	B	401	35/35	0.98	0.10	-0.42	20,23,26,30	0
2	STU	A	401	35/35	0.98	0.10	-0.45	16,22,24,25	0
2	STU	C	401	35/35	0.98	0.11	-0.48	23,27,31,33	0
2	STU	E	401	35/35	0.96	0.10	-0.52	31,36,43,44	0
2	STU	F	401	35/35	0.97	0.09	-0.53	25,29,35,37	0
3	EDO	C	404	4/4	0.98	0.08	-1.41	39,43,46,50	0
3	EDO	F	402	4/4	0.85	0.14	-	61,62,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.