



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3UIT
Title : Overall structure of Patj/Pals1/Mals complex
Authors : Zhang, J.; Yang, X.; Long, J.; Shen, Y.
Deposited on : 2011-11-06
Resolution : 2.05 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

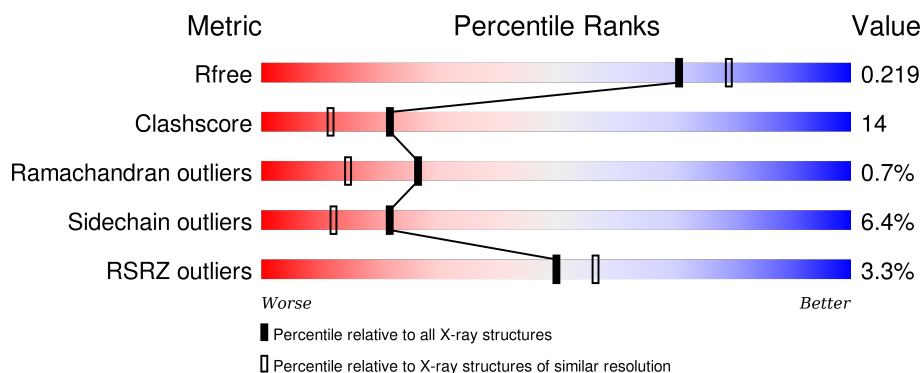
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	265	<div> <div>3%</div> <div>72% 21% . .</div> </div>
1	B	265	<div> <div>4%</div> <div>67% 25% . 5%</div> </div>
1	C	265	<div> <div>3%</div> <div>71% 23% . .</div> </div>
1	D	265	<div> <div>3%</div> <div>71% 22% . .</div> </div>

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
2	ACT	A	1428	-	-	X	-
2	ACT	A	267	-	-	-	X
2	ACT	A	271	-	-	-	X
2	ACT	A	272	-	-	-	X
2	ACT	B	1428	-	-	X	X
2	ACT	B	267	-	-	X	X
2	ACT	B	269	-	-	X	X
2	ACT	C	266	-	-	-	X
2	ACT	D	1428	-	-	X	-
2	ACT	D	266	-	-	-	X
2	ACT	D	267	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9047 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 InaD-like protein, MAGUK p55 subfamily member 5, Protein lin-7 homolog B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2027	1288	353	382	4			
1	B	253	Total	C	N	O	S	0	0	0
			2016	1281	351	380	4			
1	C	255	Total	C	N	O	S	0	0	0
			2020	1283	351	382	4			
1	D	257	Total	C	N	O	S	0	0	0
			2040	1296	355	385	4			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	-	LINKER	UNP Q63ZW7
A	70	GLU	-	LINKER	UNP Q63ZW7
A	71	VAL	-	LINKER	UNP Q63ZW7
A	72	LEU	-	LINKER	UNP Q63ZW7
A	73	PHE	-	LINKER	UNP Q63ZW7
A	74	GLN	-	LINKER	UNP Q63ZW7
A	75	GLY	-	LINKER	UNP Q63ZW7
A	76	PRO	-	LINKER	UNP Q63ZW7
A	191	GLY	-	LINKER	UNP Q9Z252
A	192	GLY	-	LINKER	UNP Q9Z252
A	193	GLY	-	LINKER	UNP Q9Z252
A	194	LEU	-	LINKER	UNP Q9Z252
A	195	GLU	-	LINKER	UNP Q9Z252
A	196	VAL	-	LINKER	UNP Q9Z252
A	197	LEU	-	LINKER	UNP Q9Z252
A	198	PHE	-	LINKER	UNP Q9Z252
A	199	GLN	-	LINKER	UNP Q9Z252
A	200	GLY	-	LINKER	UNP Q9Z252
A	201	PRO	-	LINKER	UNP Q9Z252
B	69	LEU	-	LINKER	UNP Q63ZW7

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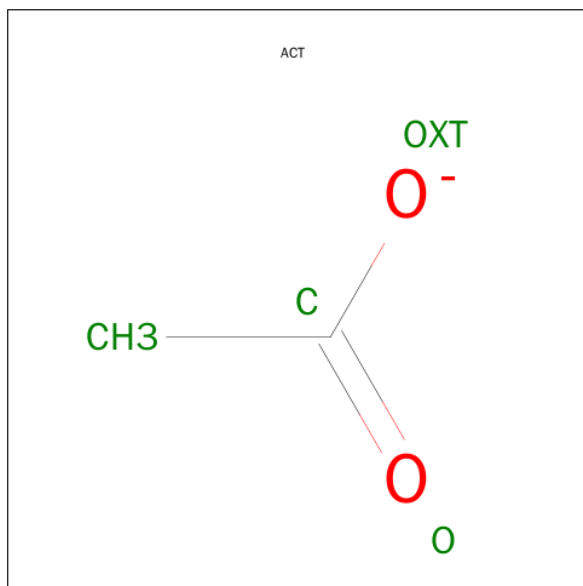
Chain	Residue	Modelled	Actual	Comment	Reference
B	70	GLU	-	LINKER	UNP Q63ZW7
B	71	VAL	-	LINKER	UNP Q63ZW7
B	72	LEU	-	LINKER	UNP Q63ZW7
B	73	PHE	-	LINKER	UNP Q63ZW7
B	74	GLN	-	LINKER	UNP Q63ZW7
B	75	GLY	-	LINKER	UNP Q63ZW7
B	76	PRO	-	LINKER	UNP Q63ZW7
B	191	GLY	-	LINKER	UNP Q9Z252
B	192	GLY	-	LINKER	UNP Q9Z252
B	193	GLY	-	LINKER	UNP Q9Z252
B	194	LEU	-	LINKER	UNP Q9Z252
B	195	GLU	-	LINKER	UNP Q9Z252
B	196	VAL	-	LINKER	UNP Q9Z252
B	197	LEU	-	LINKER	UNP Q9Z252
B	198	PHE	-	LINKER	UNP Q9Z252
B	199	GLN	-	LINKER	UNP Q9Z252
B	200	GLY	-	LINKER	UNP Q9Z252
B	201	PRO	-	LINKER	UNP Q9Z252
C	69	LEU	-	LINKER	UNP Q63ZW7
C	70	GLU	-	LINKER	UNP Q63ZW7
C	71	VAL	-	LINKER	UNP Q63ZW7
C	72	LEU	-	LINKER	UNP Q63ZW7
C	73	PHE	-	LINKER	UNP Q63ZW7
C	74	GLN	-	LINKER	UNP Q63ZW7
C	75	GLY	-	LINKER	UNP Q63ZW7
C	76	PRO	-	LINKER	UNP Q63ZW7
C	191	GLY	-	LINKER	UNP Q9Z252
C	192	GLY	-	LINKER	UNP Q9Z252
C	193	GLY	-	LINKER	UNP Q9Z252
C	194	LEU	-	LINKER	UNP Q9Z252
C	195	GLU	-	LINKER	UNP Q9Z252
C	196	VAL	-	LINKER	UNP Q9Z252
C	197	LEU	-	LINKER	UNP Q9Z252
C	198	PHE	-	LINKER	UNP Q9Z252
C	199	GLN	-	LINKER	UNP Q9Z252
C	200	GLY	-	LINKER	UNP Q9Z252
C	201	PRO	-	LINKER	UNP Q9Z252
D	69	LEU	-	LINKER	UNP Q63ZW7
D	70	GLU	-	LINKER	UNP Q63ZW7
D	71	VAL	-	LINKER	UNP Q63ZW7
D	72	LEU	-	LINKER	UNP Q63ZW7
D	73	PHE	-	LINKER	UNP Q63ZW7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	74	GLN	-	LINKER	UNP Q63ZW7
D	75	GLY	-	LINKER	UNP Q63ZW7
D	76	PRO	-	LINKER	UNP Q63ZW7
D	191	GLY	-	LINKER	UNP Q9Z252
D	192	GLY	-	LINKER	UNP Q9Z252
D	193	GLY	-	LINKER	UNP Q9Z252
D	194	LEU	-	LINKER	UNP Q9Z252
D	195	GLU	-	LINKER	UNP Q9Z252
D	196	VAL	-	LINKER	UNP Q9Z252
D	197	LEU	-	LINKER	UNP Q9Z252
D	198	PHE	-	LINKER	UNP Q9Z252
D	199	GLN	-	LINKER	UNP Q9Z252
D	200	GLY	-	LINKER	UNP Q9Z252
D	201	PRO	-	LINKER	UNP Q9Z252

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	270	Total O 270 270	0	0
3	B	194	Total O 194 194	0	0
3	C	178	Total O 178 178	0	0

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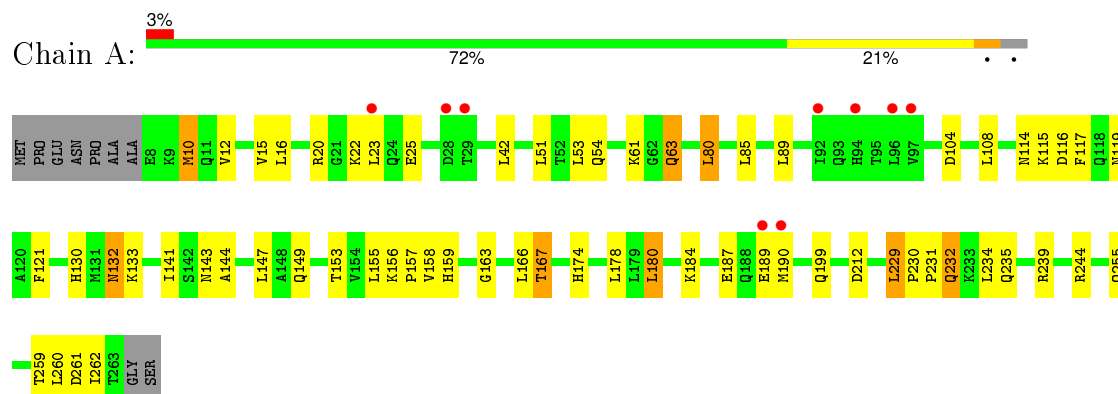
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	222	Total	O	0	0
			222	222		

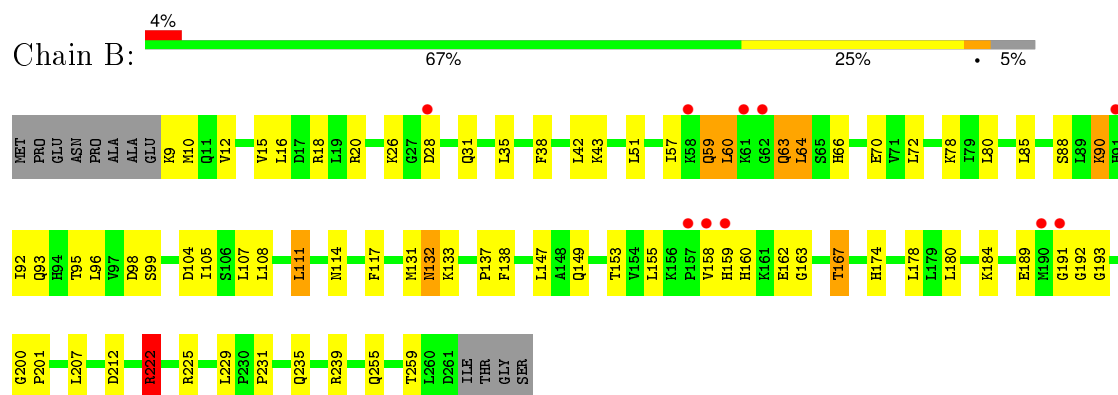
3 Residue-property plots

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.

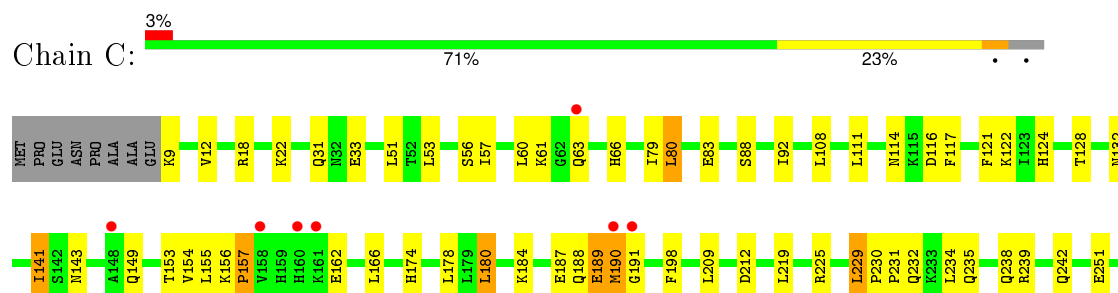
- Molecule 1: InaD-like protein, MAGUK p55 subfamily member 5, Protein lin-7 homolog B



- Molecule 1: InaD-like protein, MAGUK p55 subfamily member 5, Protein lin-7 homolog B

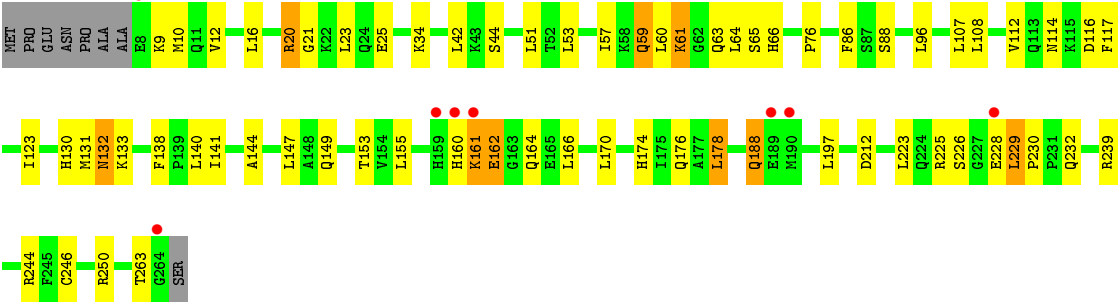


- Molecule 1: InaD-like protein, MAGUK p55 subfamily member 5, Protein lin-7 homolog B





● Molecule 1: InaD-like protein, MAGUK p55 subfamily member 5, Protein lin-7 homolog B



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.19Å 145.19Å 202.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.86 – 2.05 38.86 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.86-2.05) 96.6 (38.86-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.180 , 0.221 0.177 , 0.219	Depositor DCC
R_{free} test set	3880 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 79191 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9047	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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, 0.375 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: ACT

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	0.36	0/2059	0.54	0/2786
1	B	0.36	0/2048	0.78	1/2770 (0.0%)
1	C	0.36	0/2052	0.50	0/2778
1	D	0.38	0/2072	0.55	2/2803 (0.1%)
All	All	0.36	0/8231	0.60	3/11137 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-30.86	104.87	120.30
1	D	20	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	D	20	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	222	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2027	0	2072	65	0
1	B	2016	0	2072	64	2
1	C	2020	0	2064	56	0
1	D	2040	0	2095	69	0
2	A	32	0	24	4	0
2	B	20	0	15	8	0
2	C	8	0	6	1	0
2	D	20	0	15	10	0
3	A	270	0	0	10	0
3	B	194	0	0	6	0
3	C	178	0	0	3	0
3	D	222	0	0	1	0
All	All	9047	0	8363	231	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 14.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HD3	2:A:1428:ACT:H2	1.40	1.03
1:D:20:ARG:HH12	2:D:1428:ACT:H1	1.22	1.02
1:A:130:HIS:HB3	1:D:131:MET:CE	1.95	0.96
2:A:1428:ACT:H1	3:C:306:HOH:O	1.70	0.90
1:B:9:LYS:HZ3	2:B:269:ACT:H2	1.37	0.88
1:A:130:HIS:HB3	1:D:131:MET:HE1	1.52	0.88
1:A:80:LEU:HD13	1:A:121:PHE:HZ	1.41	0.86
1:C:187:GLU:HG3	1:C:190:MET:SD	2.18	0.84
1:D:63:GLN:HA	2:D:267:ACT:H3	1.59	0.84
1:D:114:ASN:HD22	1:D:117:PHE:H	1.24	0.84
1:D:16:LEU:O	1:D:20:ARG:HD2	1.78	0.84
1:D:123:ILE:HG12	2:D:267:ACT:H2	1.58	0.83
1:D:65:SER:H	2:D:267:ACT:H1	1.43	0.83
1:A:114:ASN:HD22	1:A:117:PHE:H	1.23	0.82
1:A:244:ARG:HH11	2:A:1428:ACT:H2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASN:HD22	1:C:117:PHE:H	1.24	0.80
1:B:35:LEU:HD11	1:B:92:ILE:HD11	1.64	0.79
1:C:235:GLN:NE2	1:C:239:ARG:HE	1.81	0.79
1:A:130:HIS:HB3	1:D:131:MET:HE3	1.68	0.76
1:B:57:ILE:HD11	1:C:198:PHE:HB3	1.68	0.74
1:B:16:LEU:O	1:B:20:ARG:HD3	1.89	0.72
1:A:163:GLY:O	1:A:167:THR:HG23	1.88	0.72
1:A:244:ARG:HH11	2:A:1428:ACT:CH3	2.03	0.72
1:B:138:PHE:H	2:B:1428:ACT:H3	1.53	0.72
1:B:10:MET:HG2	1:B:12:VAL:HG12	1.72	0.70
1:C:229:LEU:HD11	1:C:234:LEU:HD11	1.72	0.70
1:D:20:ARG:NH1	2:D:1428:ACT:H1	2.02	0.70
1:D:16:LEU:O	1:D:20:ARG:CD	2.39	0.70
1:C:114:ASN:HD21	1:C:116:ASP:HB2	1.57	0.70
1:A:199:GLN:HG2	3:A:761:HOH:O	1.92	0.69
1:B:92:ILE:HG22	1:B:105:ILE:HD11	1.74	0.68
1:B:114:ASN:HD22	1:B:117:PHE:H	1.39	0.68
1:B:235:GLN:NE2	1:B:239:ARG:HE	1.92	0.68
1:B:137:PRO:HA	2:B:1428:ACT:H1	1.75	0.67
1:B:35:LEU:HD11	1:B:92:ILE:CD1	2.25	0.67
1:A:167:THR:HG21	3:A:750:HOH:O	1.94	0.67
1:A:54:GLN:NE2	1:A:119:ASN:HD22	1.93	0.66
1:D:34:LYS:HE3	1:D:88:SER:OG	1.95	0.66
1:B:64:LEU:HD21	1:C:256:LEU:HD21	1.77	0.65
1:A:229:LEU:HD11	1:A:234:LEU:HD11	1.78	0.65
1:D:226:SER:OG	1:D:228:GLU:HG2	1.97	0.65
1:B:163:GLY:O	1:B:167:THR:HG23	1.97	0.65
1:C:262:ILE:O	1:C:263:THR:HG22	1.97	0.64
1:A:25:GLU:HA	1:C:225:ARG:HA	1.78	0.64
1:B:225:ARG:HA	1:D:25:GLU:HA	1.79	0.63
1:A:232:GLN:NE2	1:A:232:GLN:H	1.96	0.63
1:A:235:GLN:NE2	1:A:239:ARG:HE	1.96	0.63
1:D:130:HIS:HB2	1:D:131:MET:CE	2.30	0.62
1:D:174:HIS:HE1	1:D:212:ASP:OD2	1.81	0.62
1:D:162:GLU:HB3	1:D:223:LEU:HD21	1.82	0.62
1:D:114:ASN:HD21	1:D:116:ASP:HB2	1.65	0.62
1:A:174:HIS:HE1	1:A:212:ASP:OD2	1.81	0.61
1:C:229:LEU:HB2	1:C:230:PRO:HD2	1.83	0.61
2:B:1428:ACT:H2	3:B:274:HOH:O	2.01	0.61
1:A:80:LEU:HD12	1:A:80:LEU:H	1.66	0.60
3:A:819:HOH:O	1:C:33:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LYS:NZ	2:B:269:ACT:H2	2.13	0.59
1:A:187:GLU:OE1	1:A:190:MET:HB2	2.01	0.59
1:B:16:LEU:O	1:B:20:ARG:CD	2.50	0.59
1:C:174:HIS:CD2	1:C:174:HIS:H	2.21	0.59
1:C:128:THR:HG22	3:C:316:HOH:O	2.02	0.59
1:D:10:MET:HG2	1:D:12:VAL:HG12	1.84	0.58
1:D:130:HIS:HB2	1:D:131:MET:HE2	1.85	0.58
1:A:143:ASN:HB2	3:A:748:HOH:O	2.02	0.58
1:B:158:VAL:HG11	1:B:229:LEU:HD21	1.84	0.57
1:A:15:VAL:HG13	1:A:104:ASP:HB3	1.86	0.57
1:A:114:ASN:ND2	1:A:117:PHE:H	2.00	0.57
1:B:63:GLN:HG2	1:C:63:GLN:HE22	1.70	0.57
1:D:63:GLN:O	1:D:66:HIS:ND1	2.36	0.57
1:A:16:LEU:O	1:A:20:ARG:HD3	2.04	0.57
1:C:180:LEU:HD22	1:C:184:LYS:HD2	1.86	0.57
1:D:65:SER:H	2:D:267:ACT:CH3	2.15	0.57
1:A:80:LEU:HD13	1:A:121:PHE:CZ	2.32	0.57
1:D:63:GLN:CA	2:D:267:ACT:H3	2.31	0.57
1:B:26:LYS:HG2	3:B:622:HOH:O	2.05	0.56
1:A:232:GLN:HE21	1:A:232:GLN:H	1.52	0.56
1:C:155:LEU:HD11	1:C:166:LEU:HD23	1.85	0.56
1:C:154:VAL:HG12	1:C:229:LEU:HD13	1.88	0.56
1:C:174:HIS:HE1	1:C:212:ASP:OD2	1.88	0.56
1:D:161:LYS:HA	1:D:164:GLN:HB3	1.88	0.56
1:C:79:ILE:HG21	1:C:128:THR:OG1	2.07	0.55
1:A:235:GLN:HE22	1:A:239:ARG:HE	1.55	0.55
1:B:160:HIS:HB3	1:B:163:GLY:H	1.71	0.55
1:B:26:LYS:HG3	1:B:96:LEU:HD23	1.88	0.55
1:D:160:HIS:O	1:D:162:GLU:N	2.40	0.55
1:B:28:ASP:HB3	1:B:95:THR:HG21	1.89	0.55
1:B:63:GLN:O	1:B:66:HIS:CE1	2.60	0.55
1:C:255:GLN:O	1:C:259:THR:HG23	2.07	0.55
1:C:88:SER:O	1:C:92:ILE:HG12	2.05	0.55
1:D:170:LEU:O	1:D:176:GLN:NE2	2.39	0.54
1:A:85:LEU:O	1:A:89:LEU:HG	2.06	0.54
1:B:57:ILE:HD11	1:C:198:PHE:CB	2.37	0.53
1:B:20:ARG:NH2	1:D:239:ARG:HG3	2.23	0.53
1:D:114:ASN:ND2	1:D:117:PHE:H	2.02	0.53
1:A:231:PRO:HG3	1:C:22:LYS:HD3	1.91	0.53
1:B:174:HIS:HD2	3:B:810:HOH:O	1.92	0.52
1:B:80:LEU:H	1:B:80:LEU:HD23	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG13	1:B:104:ASP:HB3	1.92	0.52
1:B:92:ILE:HG22	1:B:105:ILE:CD1	2.40	0.52
1:B:174:HIS:HE1	1:B:212:ASP:OD2	1.93	0.52
1:D:9:LYS:HD3	1:D:9:LYS:O	2.10	0.52
1:B:18:ARG:HG2	1:D:232:GLN:HB2	1.92	0.52
1:A:16:LEU:O	1:A:20:ARG:CD	2.57	0.51
1:C:31:GLN:HB2	1:C:92:ILE:HD11	1.92	0.51
1:A:260:LEU:HD22	1:D:59:GLN:HB3	1.92	0.51
1:D:228:GLU:HG3	1:D:229:LEU:HG	1.93	0.51
1:D:160:HIS:C	1:D:162:GLU:H	2.14	0.51
1:C:114:ASN:ND2	1:C:117:PHE:H	2.02	0.50
1:C:141:ILE:HG23	1:C:143:ASN:H	1.76	0.50
1:C:124:HIS:O	1:C:128:THR:HG23	2.12	0.50
1:D:61:LYS:HA	3:D:887:HOH:O	2.11	0.50
1:A:23:LEU:HD13	3:A:347:HOH:O	2.11	0.50
1:D:155:LEU:HD11	1:D:166:LEU:HD23	1.92	0.50
1:A:80:LEU:HD12	3:A:322:HOH:O	2.12	0.50
1:B:90:LYS:HE2	1:B:93:GLN:NE2	2.27	0.50
1:C:83:GLU:H	1:C:83:GLU:CD	2.15	0.49
1:A:132:ASN:HD21	1:A:133:LYS:NZ	2.11	0.49
1:A:229:LEU:HB2	1:A:230:PRO:HD2	1.95	0.49
1:C:63:GLN:O	1:C:66:HIS:CE1	2.66	0.49
1:A:22:LYS:HD3	1:C:231:PRO:HG3	1.94	0.49
1:A:174:HIS:H	1:A:174:HIS:CD2	2.29	0.49
1:A:63:GLN:CD	1:D:63:GLN:HE22	2.16	0.48
1:C:149:GLN:O	1:C:153:THR:HG23	2.13	0.48
1:A:232:GLN:HG3	1:C:18:ARG:HB2	1.96	0.48
1:C:60:LEU:O	1:C:61:LYS:HE2	2.14	0.48
1:C:229:LEU:CD1	1:C:234:LEU:HD11	2.40	0.48
1:B:155:LEU:O	1:B:158:VAL:HG22	2.13	0.48
1:C:189:GLU:C	1:C:191:GLY:H	2.17	0.48
1:A:174:HIS:CE1	1:A:212:ASP:OD2	2.65	0.48
1:A:187:GLU:HG2	3:A:807:HOH:O	2.12	0.48
1:B:63:GLN:O	1:B:66:HIS:ND1	2.47	0.48
1:A:261:ASP:O	1:D:59:GLN:HG3	2.14	0.48
1:A:260:LEU:HD23	1:D:60:LEU:HD23	1.96	0.47
1:D:107:LEU:HD23	1:D:107:LEU:C	2.34	0.47
1:B:149:GLN:O	1:B:153:THR:HG23	2.13	0.47
1:C:156:LYS:N	1:C:157:PRO:HD2	2.30	0.47
1:D:107:LEU:HD23	1:D:107:LEU:O	2.14	0.47
1:C:235:GLN:HE22	1:C:239:ARG:HE	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PHE:CZ	1:D:112:VAL:HG12	2.50	0.47
1:A:156:LYS:HB3	1:A:157:PRO:HD3	1.96	0.47
1:B:57:ILE:HG22	1:B:60:LEU:N	2.29	0.47
1:A:255:GLN:O	1:A:259:THR:HG23	2.15	0.47
1:A:229:LEU:CD1	1:A:234:LEU:HD11	2.45	0.46
1:C:9:LYS:O	1:C:12:VAL:HG12	2.15	0.46
1:B:70:GLU:HG3	1:B:131:MET:CE	2.46	0.46
1:D:23:LEU:HG	1:D:96:LEU:HD11	1.96	0.46
1:C:80:LEU:O	1:C:121:PHE:HE2	1.99	0.46
1:C:251:GLU:HG2	2:C:266:ACT:CH3	2.46	0.46
1:C:56:SER:HB2	1:C:57:ILE:HD12	1.97	0.46
1:D:61:LYS:HE3	1:D:61:LYS:HB2	1.64	0.46
1:B:111:LEU:HD22	1:B:117:PHE:CD1	2.51	0.45
1:D:174:HIS:CE1	1:D:212:ASP:OD2	2.65	0.45
1:B:158:VAL:HG23	1:B:160:HIS:H	1.80	0.45
2:B:267:ACT:H2	1:D:138:PHE:H	1.81	0.45
1:B:132:ASN:ND2	1:B:133:LYS:HD2	2.32	0.45
1:B:155:LEU:HD12	1:B:167:THR:HG22	1.99	0.45
1:A:22:LYS:HD2	1:A:22:LYS:HA	1.70	0.45
1:A:141:ILE:HD11	1:A:144:ALA:HA	1.99	0.45
1:C:238:GLN:HG2	1:C:242:GLN:OE1	2.17	0.45
1:D:229:LEU:HB2	1:D:230:PRO:HD2	1.99	0.45
1:B:59:GLN:NE2	1:B:59:GLN:H	2.14	0.44
1:B:207:LEU:HD21	3:B:874:HOH:O	2.17	0.44
1:C:188:GLN:OE1	1:D:188:GLN:HG3	2.18	0.44
1:B:57:ILE:O	1:B:57:ILE:HG22	2.18	0.44
1:D:132:ASN:HD21	1:D:133:LYS:NZ	2.15	0.44
1:B:64:LEU:HD21	1:C:256:LEU:CD2	2.48	0.44
1:A:187:GLU:C	1:A:189:GLU:H	2.22	0.43
2:B:267:ACT:CH3	1:D:138:PHE:H	2.31	0.43
1:C:122:LYS:HD2	1:C:122:LYS:N	2.33	0.43
1:C:162:GLU:CG	1:C:219:LEU:HD22	2.48	0.43
1:B:78:LYS:HB3	1:B:78:LYS:HE2	1.76	0.43
1:C:153:THR:O	1:C:156:LYS:HB2	2.18	0.43
1:D:130:HIS:HB2	1:D:131:MET:HE1	1.97	0.43
1:D:65:SER:CB	2:D:267:ACT:H1	2.48	0.43
3:A:761:HOH:O	1:D:57:ILE:HD11	2.18	0.43
1:A:10:MET:HE2	1:A:10:MET:HB3	1.97	0.43
1:A:184:LYS:HB3	1:A:184:LYS:HE2	1.76	0.43
3:A:373:HOH:O	1:C:232:GLN:HG2	2.18	0.43
1:C:141:ILE:HD12	3:C:320:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HG21	3:A:635:HOH:O	2.19	0.42
1:A:155:LEU:HD11	1:A:166:LEU:HD23	2.00	0.42
1:A:25:GLU:CA	1:C:225:ARG:HA	2.48	0.42
1:D:160:HIS:C	1:D:162:GLU:N	2.72	0.42
1:B:43:LYS:HE2	1:D:140:LEU:O	2.19	0.42
1:D:65:SER:N	2:D:267:ACT:H1	2.21	0.42
1:B:80:LEU:HD11	1:B:85:LEU:HD13	2.02	0.42
1:A:132:ASN:HD21	1:A:133:LYS:HZ2	1.67	0.42
1:B:184:LYS:HE3	1:B:193:GLY:HA2	2.01	0.42
1:A:156:LYS:HE2	1:A:156:LYS:HB3	1.78	0.42
1:B:231:PRO:HB2	1:D:21:GLY:HA3	2.00	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD12	1.86	0.42
1:A:130:HIS:CB	1:D:131:MET:HE3	2.45	0.42
1:B:174:HIS:H	1:B:174:HIS:CD2	2.37	0.42
2:B:267:ACT:O	1:D:244:ARG:HD3	2.19	0.42
3:B:323:HOH:O	1:C:188:GLN:HA	2.20	0.42
1:A:149:GLN:O	1:A:153:THR:HG23	2.19	0.42
1:A:132:ASN:HD22	1:A:132:ASN:H	1.68	0.42
1:D:44:SER:HB2	1:D:76:PRO:HD3	2.02	0.42
1:A:114:ASN:HD21	1:A:116:ASP:HB2	1.85	0.41
1:B:235:GLN:HE22	1:B:239:ARG:HE	1.66	0.41
1:D:20:ARG:HH12	2:D:1428:ACT:CH3	2.11	0.41
1:D:132:ASN:HD22	1:D:132:ASN:C	2.23	0.41
1:C:61:LYS:HA	1:C:61:LYS:HE2	2.02	0.41
1:D:141:ILE:HD11	1:D:144:ALA:HA	2.03	0.41
1:D:246:CYS:O	1:D:250:ARG:HG3	2.20	0.41
1:C:262:ILE:O	1:C:263:THR:CG2	2.67	0.41
1:B:174:HIS:CE1	1:B:212:ASP:OD2	2.73	0.41
1:A:115:LYS:HA	1:A:115:LYS:HD3	1.72	0.41
1:B:160:HIS:HD2	1:B:162:GLU:HB2	1.84	0.41
1:A:10:MET:HE2	1:A:12:VAL:CG1	2.51	0.41
1:A:180:LEU:HD22	1:A:184:LYS:HG3	2.02	0.41
1:B:201:PRO:HA	3:B:811:HOH:O	2.20	0.41
1:B:191:GLY:HA2	1:B:192:GLY:HA3	1.87	0.41
1:B:66:HIS:CE1	1:C:259:THR:HG21	2.56	0.41
1:B:31:GLN:NE2	1:B:88:SER:HA	2.36	0.41
1:D:239:ARG:HD3	1:D:239:ARG:HA	1.87	0.41
1:A:187:GLU:O	1:A:189:GLU:HG2	2.20	0.41
1:B:38:PHE:CG	1:B:85:LEU:HD11	2.56	0.41
1:D:174:HIS:CD2	1:D:174:HIS:H	2.38	0.41
1:B:200:GLY:HA3	1:B:201:PRO:HD2	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:O	1:A:159:HIS:HB2	2.21	0.41
1:B:38:PHE:CE1	1:B:85:LEU:HD21	2.57	0.40
1:D:107:LEU:CD2	1:D:107:LEU:C	2.90	0.40
1:B:255:GLN:O	1:B:259:THR:HG23	2.21	0.40
1:D:160:HIS:H	1:D:160:HIS:CD2	2.38	0.40
1:C:189:GLU:O	1:C:191:GLY:N	2.52	0.40
1:D:149:GLN:O	1:D:153:THR:HG23	2.21	0.40
1:A:190:MET:O	1:A:190:MET:HG3	2.21	0.40
1:C:80:LEU:O	1:C:121:PHE:CE2	2.75	0.40
1:D:178:LEU:HA	1:D:197:LEU:HD21	2.03	0.40
1:B:98:ASP:OD1	1:B:99:SER:N	2.55	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:B:222:ARG:CZ	1:B:222:ARG:NH2[11_455]	1.33	0.87
1:B:222:ARG:NE	1:B:222:ARG:NH2[11_455]	2.11	0.09

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	254/265 (96%)	245 (96%)	8 (3%)	1 (0%)	39	28
1	B	251/265 (95%)	237 (94%)	12 (5%)	2 (1%)	24	12
1	C	253/265 (96%)	242 (96%)	9 (4%)	2 (1%)	24	12
1	D	255/265 (96%)	245 (96%)	8 (3%)	2 (1%)	24	12
All	All	1013/1060 (96%)	969 (96%)	37 (4%)	7 (1%)	26	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	MET
1	D	161	LYS
1	B	63	GLN
1	C	157	PRO
1	D	263	THR
1	B	159	HIS
1	A	262	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	227/237 (96%)	212 (93%)	15 (7%)	21	11
1	B	228/237 (96%)	212 (93%)	16 (7%)	19	10
1	C	227/237 (96%)	214 (94%)	13 (6%)	25	15
1	D	230/237 (97%)	216 (94%)	14 (6%)	23	13
All	All	912/948 (96%)	854 (94%)	58 (6%)	22	12

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	42	LEU
1	A	51	LEU
1	A	53	LEU
1	A	61	LYS
1	A	63	GLN
1	A	80	LEU
1	A	108	LEU
1	A	132	ASN
1	A	147	LEU
1	A	167	THR
1	A	178	LEU
1	A	180	LEU
1	A	229	LEU
1	A	232	GLN

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Mol	Chain	Res	Type
1	B	42	LEU
1	B	51	LEU
1	B	59	GLN
1	B	60	LEU
1	B	64	LEU
1	B	72	LEU
1	B	90	LYS
1	B	107	LEU
1	B	108	LEU
1	B	111	LEU
1	B	132	ASN
1	B	147	LEU
1	B	167	THR
1	B	178	LEU
1	B	180	LEU
1	B	189	GLU
1	C	51	LEU
1	C	53	LEU
1	C	80	LEU
1	C	108	LEU
1	C	111	LEU
1	C	132	ASN
1	C	141	ILE
1	C	178	LEU
1	C	180	LEU
1	C	189	GLU
1	C	209	LEU
1	C	229	LEU
1	C	263	THR
1	D	42	LEU
1	D	51	LEU
1	D	53	LEU
1	D	59	GLN
1	D	61	LYS
1	D	64	LEU
1	D	108	LEU
1	D	132	ASN
1	D	147	LEU
1	D	162	GLU
1	D	178	LEU
1	D	188	GLN
1	D	225	ARG

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Mol	Chain	Res	Type
1	D	229	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	31	GLN
1	A	54	GLN
1	A	63	GLN
1	A	91	HIS
1	A	114	ASN
1	A	132	ASN
1	A	149	GLN
1	A	174	HIS
1	A	232	GLN
1	A	235	GLN
1	B	11	GLN
1	B	31	GLN
1	B	59	GLN
1	B	91	HIS
1	B	93	GLN
1	B	114	ASN
1	B	132	ASN
1	B	160	HIS
1	B	174	HIS
1	B	235	GLN
1	C	31	GLN
1	C	63	GLN
1	C	114	ASN
1	C	132	ASN
1	C	152	GLN
1	C	174	HIS
1	C	235	GLN
1	D	31	GLN
1	D	54	GLN
1	D	63	GLN
1	D	114	ASN
1	D	132	ASN
1	D	174	HIS
1	D	176	GLN
1	D	188	GLN

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 ⓘ

20 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	ACT	A	1428	-	1,3,3	0.38	0	0,3,3	0.00	-
2	ACT	A	266	-	1,3,3	1.57	0	0,3,3	0.00	-
2	ACT	A	267	-	1,3,3	1.38	0	0,3,3	0.00	-
2	ACT	A	268	-	1,3,3	1.14	0	0,3,3	0.00	-
2	ACT	A	269	-	1,3,3	1.20	0	0,3,3	0.00	-
2	ACT	A	270	-	1,3,3	1.24	0	0,3,3	0.00	-
2	ACT	A	271	-	1,3,3	1.27	0	0,3,3	0.00	-
2	ACT	A	272	-	1,3,3	1.40	0	0,3,3	0.00	-
2	ACT	B	1428	-	1,3,3	0.01	0	0,3,3	0.00	-
2	ACT	B	266	-	1,3,3	1.34	0	0,3,3	0.00	-
2	ACT	B	267	-	1,3,3	1.09	0	0,3,3	0.00	-
2	ACT	B	268	-	1,3,3	1.52	0	0,3,3	0.00	-
2	ACT	B	269	-	1,3,3	1.02	0	0,3,3	0.00	-
2	ACT	C	1428	-	1,3,3	1.03	0	0,3,3	0.00	-
2	ACT	C	266	-	1,3,3	1.55	0	0,3,3	0.00	-
2	ACT	D	1428	-	1,3,3	0.17	0	0,3,3	0.00	-
2	ACT	D	266	-	1,3,3	1.39	0	0,3,3	0.00	-
2	ACT	D	267	-	1,3,3	0.79	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	D	268	-	1,3,3	1.24	0	0,3,3	0.00	-
2	ACT	D	269	-	1,3,3	1.31	0	0,3,3	0.00	-

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	ACT	A	1428	-	-	0/0/0/0	0/0/0/0
2	ACT	A	266	-	-	0/0/0/0	0/0/0/0
2	ACT	A	267	-	-	0/0/0/0	0/0/0/0
2	ACT	A	268	-	-	0/0/0/0	0/0/0/0
2	ACT	A	269	-	-	0/0/0/0	0/0/0/0
2	ACT	A	270	-	-	0/0/0/0	0/0/0/0
2	ACT	A	271	-	-	0/0/0/0	0/0/0/0
2	ACT	A	272	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1428	-	-	0/0/0/0	0/0/0/0
2	ACT	B	266	-	-	0/0/0/0	0/0/0/0
2	ACT	B	267	-	-	0/0/0/0	0/0/0/0
2	ACT	B	268	-	-	0/0/0/0	0/0/0/0
2	ACT	B	269	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1428	-	-	0/0/0/0	0/0/0/0
2	ACT	C	266	-	-	0/0/0/0	0/0/0/0
2	ACT	D	1428	-	-	0/0/0/0	0/0/0/0
2	ACT	D	266	-	-	0/0/0/0	0/0/0/0
2	ACT	D	267	-	-	0/0/0/0	0/0/0/0
2	ACT	D	268	-	-	0/0/0/0	0/0/0/0
2	ACT	D	269	-	-	0/0/0/0	0/0/0/0

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.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1428	ACT	4	0
2	B	1428	ACT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	267	ACT	3	0
2	B	269	ACT	2	0
2	C	266	ACT	1	0
2	D	1428	ACT	3	0
2	D	267	ACT	7	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	256/265 (96%)	-0.27	9 (3%) 48 54	18, 34, 68, 118	0
1	B	253/265 (95%)	-0.06	10 (3%) 42 48	20, 36, 81, 137	0
1	C	255/265 (96%)	-0.10	7 (2%) 58 64	19, 38, 79, 122	0
1	D	257/265 (96%)	-0.28	8 (3%) 52 60	19, 32, 74, 140	0
All	All	1021/1060 (96%)	-0.18	34 (3%) 50 57	18, 34, 76, 140	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	VAL	4.4
1	D	190	MET	4.0
1	D	159	HIS	3.8
1	A	97	VAL	3.8
1	B	159	HIS	3.7
1	D	8	GLU	3.7
1	B	157	PRO	3.5
1	D	161	LYS	3.3
1	D	189	GLU	3.3
1	B	62	GLY	3.1
1	C	160	HIS	3.0
1	D	160	HIS	3.0
1	C	63	GLN	2.9
1	A	189	GLU	2.9
1	A	23	LEU	2.8
1	A	190	MET	2.8
1	A	96	LEU	2.8
1	B	91	HIS	2.8
1	C	190	MET	2.7
1	B	28	ASP	2.6
1	C	158	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLY	2.5
1	C	191	GLY	2.5
1	A	94	HIS	2.4
1	B	61	LYS	2.3
1	D	228	GLU	2.3
1	A	29	THR	2.3
1	B	58	LYS	2.3
1	C	148	ALA	2.3
1	D	264	GLY	2.1
1	A	28	ASP	2.1
1	B	190	MET	2.1
1	A	92	ILE	2.1
1	C	161	LYS	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
2	ACT	A	271	4/4	0.94	0.24	10.76	47,49,55,67	0
2	ACT	A	272	4/4	0.88	0.20	10.49	58,62,63,64	0
2	ACT	B	267	4/4	0.80	0.19	4.05	33,43,49,58	0
2	ACT	C	266	4/4	0.88	0.15	3.05	45,55,56,60	0
2	ACT	B	269	4/4	0.76	0.22	3.02	52,59,66,78	0
2	ACT	D	266	4/4	0.84	0.15	2.78	55,55,57,62	0
2	ACT	B	1428	4/4	0.92	0.16	2.50	28,32,43,54	0
2	ACT	A	267	4/4	0.86	0.19	2.29	48,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ACT	D	267	4/4	0.77	0.27	1.88	55,68,70,72	0
2	ACT	B	268	4/4	0.92	0.14	1.84	42,54,55,59	0
2	ACT	A	268	4/4	0.93	0.20	1.22	55,59,63,71	0
2	ACT	A	1428	4/4	0.92	0.13	0.29	31,38,43,47	0
2	ACT	D	268	4/4	0.90	0.18	-0.05	68,80,82,85	0
2	ACT	D	1428	4/4	0.98	0.10	-0.45	13,25,26,42	0
2	ACT	A	266	4/4	0.99	0.09	-0.58	30,32,33,39	0
2	ACT	B	266	4/4	0.97	0.09	-0.68	26,28,28,31	0
2	ACT	C	1428	4/4	0.98	0.10	-1.77	27,27,29,29	0
2	ACT	A	270	4/4	0.76	0.26	-	71,72,75,78	0
2	ACT	A	269	4/4	0.81	0.26	-	98,99,100,101	0
2	ACT	D	269	4/4	0.59	0.24	-	96,97,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.