



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:19 PM UTC

PDB ID : 3E4Z / pdb_00003e4z
Title : Crystal structure of human insulin degrading enzyme in complex with insulin-like growth factor II
Authors : Guo, Q.; Manolopoulou, M.; Tang, W.-J.
Deposited on : 2008-08-12
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

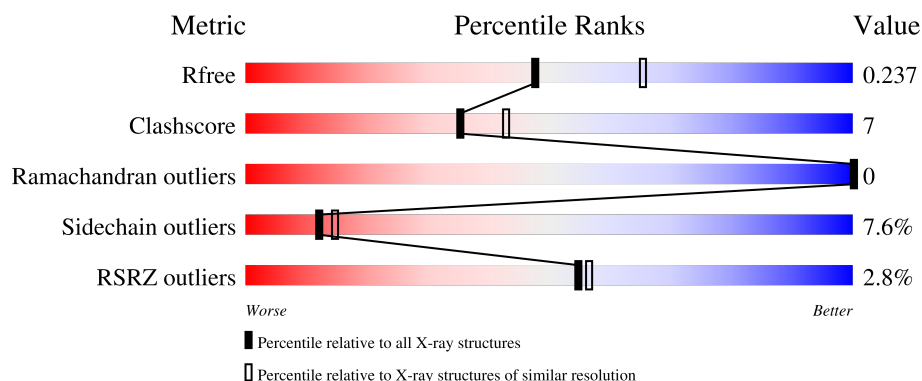
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	990	0% 78% 16% • •
1	B	990	3% 77% 17% • •
2	C	67	12% 10% • • 87%
2	D	67	12% 7% • • 87%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16411 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7783	5014	1306	1441	22			
1	B	952	Total	C	N	O	S	0	0	0
			7778	5011	1305	1440	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP Q5T5N2
A	31	HIS	-	expression tag	UNP Q5T5N2
A	32	HIS	-	expression tag	UNP Q5T5N2
A	33	HIS	-	expression tag	UNP Q5T5N2
A	34	HIS	-	expression tag	UNP Q5T5N2
A	35	HIS	-	expression tag	UNP Q5T5N2
A	36	HIS	-	expression tag	UNP Q5T5N2
A	37	ALA	-	expression tag	UNP Q5T5N2
A	38	ALA	-	expression tag	UNP Q5T5N2
A	39	GLY	-	expression tag	UNP Q5T5N2
A	40	ILE	-	expression tag	UNP Q5T5N2
A	41	PRO	-	expression tag	UNP Q5T5N2
A	110	LEU	CYS	engineered mutation	UNP Q5T5N2
A	111	GLN	GLU	engineered mutation	UNP Q5T5N2
A	171	SER	CYS	engineered mutation	UNP Q5T5N2
A	178	ALA	CYS	engineered mutation	UNP Q5T5N2
A	257	VAL	CYS	engineered mutation	UNP Q5T5N2
A	414	LEU	CYS	engineered mutation	UNP Q5T5N2
A	573	ASN	CYS	engineered mutation	UNP Q5T5N2
A	590	SER	CYS	engineered mutation	UNP Q5T5N2
A	789	SER	CYS	engineered mutation	UNP Q5T5N2
A	812	ALA	CYS	engineered mutation	UNP Q5T5N2
A	819	ALA	CYS	engineered mutation	UNP Q5T5N2
A	904	SER	CYS	engineered mutation	UNP Q5T5N2
A	908	TYR	TRP	engineered mutation	UNP Q5T5N2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	expression tag	UNP Q5T5N2
B	31	HIS	-	expression tag	UNP Q5T5N2
B	32	HIS	-	expression tag	UNP Q5T5N2
B	33	HIS	-	expression tag	UNP Q5T5N2
B	34	HIS	-	expression tag	UNP Q5T5N2
B	35	HIS	-	expression tag	UNP Q5T5N2
B	36	HIS	-	expression tag	UNP Q5T5N2
B	37	ALA	-	expression tag	UNP Q5T5N2
B	38	ALA	-	expression tag	UNP Q5T5N2
B	39	GLY	-	expression tag	UNP Q5T5N2
B	40	ILE	-	expression tag	UNP Q5T5N2
B	41	PRO	-	expression tag	UNP Q5T5N2
B	110	LEU	CYS	engineered mutation	UNP Q5T5N2
B	111	GLN	GLU	engineered mutation	UNP Q5T5N2
B	171	SER	CYS	engineered mutation	UNP Q5T5N2
B	178	ALA	CYS	engineered mutation	UNP Q5T5N2
B	257	VAL	CYS	engineered mutation	UNP Q5T5N2
B	414	LEU	CYS	engineered mutation	UNP Q5T5N2
B	573	ASN	CYS	engineered mutation	UNP Q5T5N2
B	590	SER	CYS	engineered mutation	UNP Q5T5N2
B	789	SER	CYS	engineered mutation	UNP Q5T5N2
B	812	ALA	CYS	engineered mutation	UNP Q5T5N2
B	819	ALA	CYS	engineered mutation	UNP Q5T5N2
B	904	SER	CYS	engineered mutation	UNP Q5T5N2
B	908	TYR	TRP	engineered mutation	UNP Q5T5N2

- Molecule 2 is a protein called Insulin-like growth factor II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			62	39	10	13			
2	D	9	Total	C	N	O	0	0	0
			62	39	10	13			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

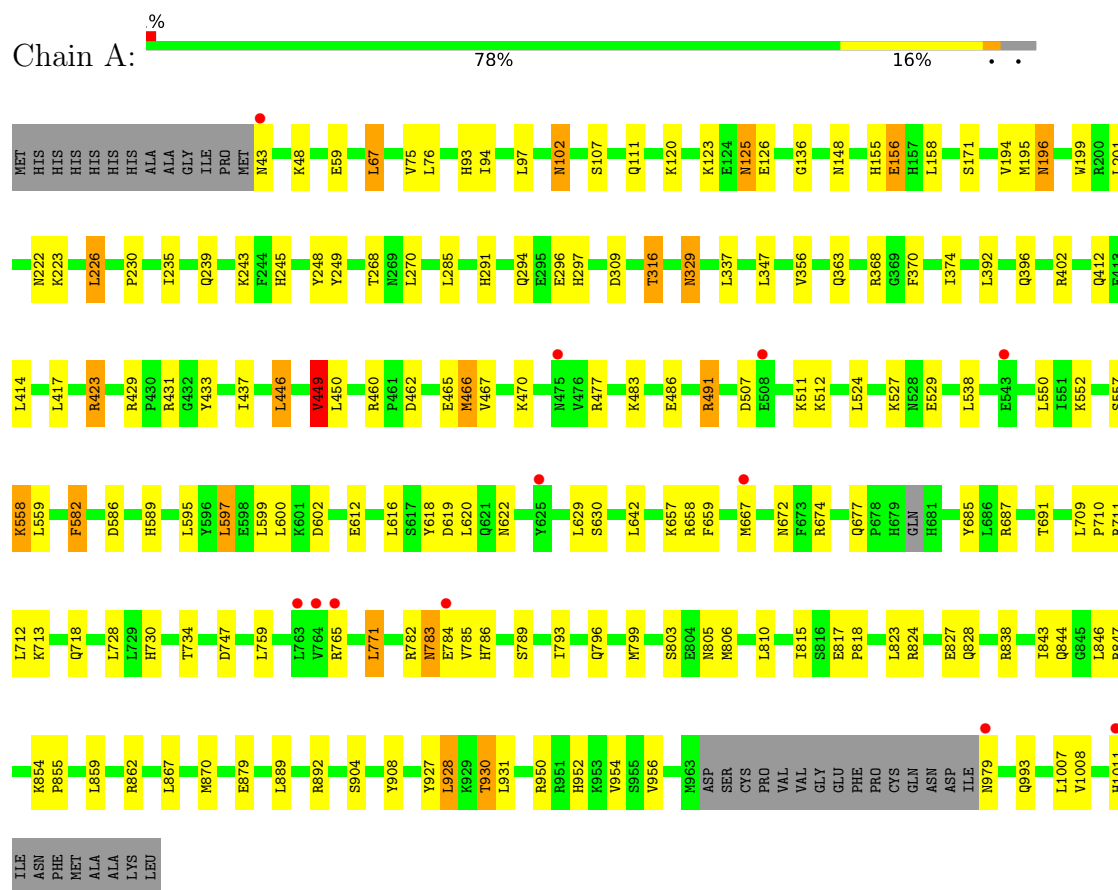
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	384	Total 384	O 384	0	0
4	B	338	Total 338	O 338	0	0
4	C	2	Total 2	O 2	0	0

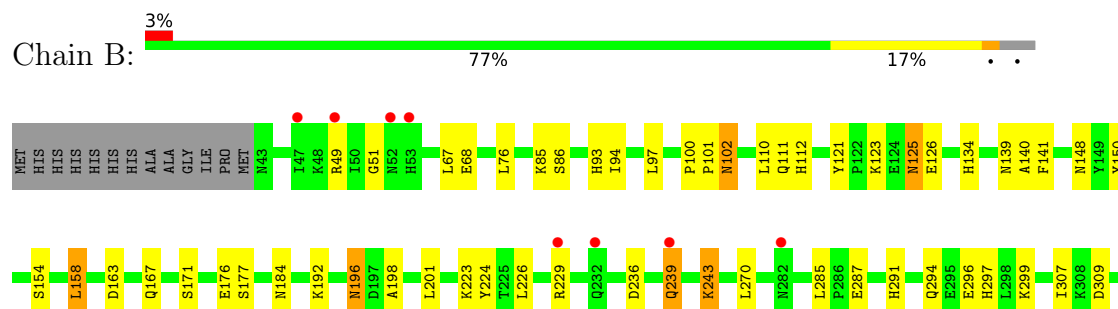
3 Residue-property plots

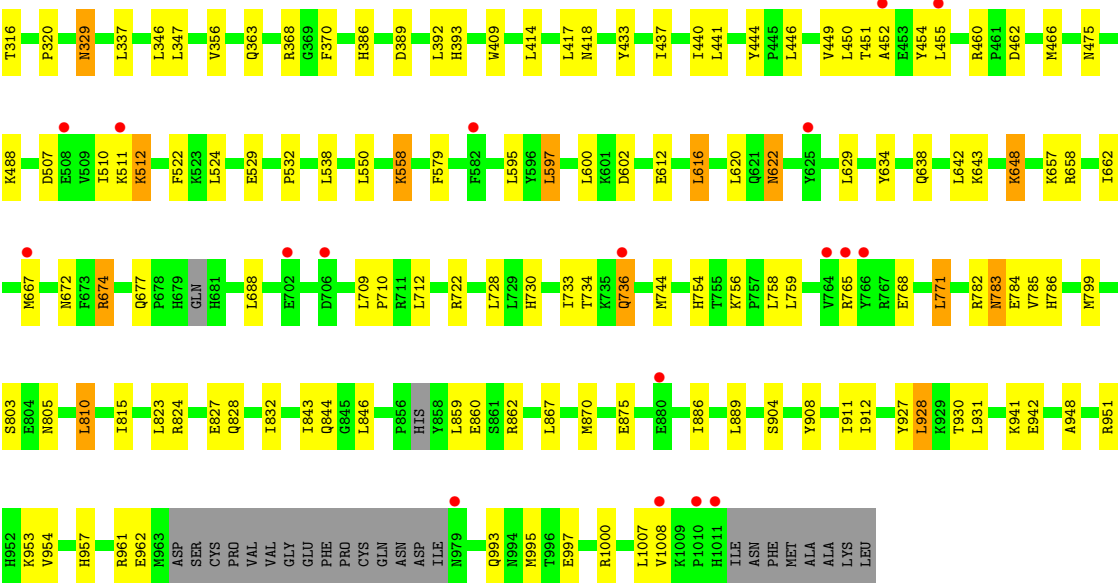
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Insulin-degrading enzyme

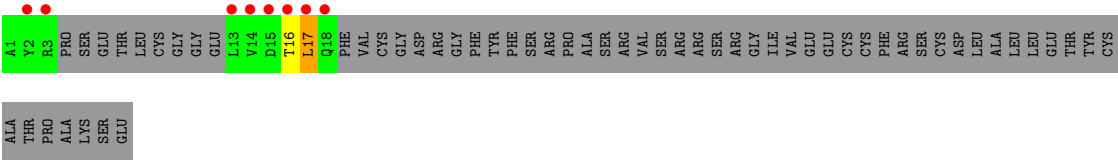


• Molecule 1: Insulin-degrading enzyme

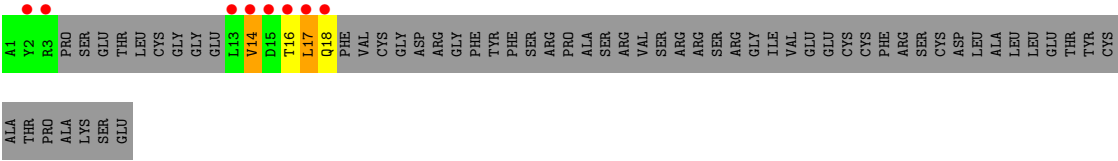




● Molecule 2: Insulin-like growth factor II



● Molecule 2: Insulin-like growth factor II



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.03Å 263.03Å 90.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.28 50.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.28) 99.7 (50.00-2.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.230 0.206 , 0.237	Depositor DCC
R_{free} test set	8139 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16411	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.68	0/7975	0.88	5/10787 (0.0%)
1	B	0.66	0/7969	0.87	1/10777 (0.0%)
2	C	0.90	0/60	1.27	0/80
2	D	0.88	0/60	0.86	0/80
All	All	0.67	0/16064	0.88	6/21724 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	VAL	CB-CA-C	-6.49	102.11	112.16
1	B	171	SER	N-CA-C	5.48	116.65	108.76
1	A	429	ARG	CA-C-N	5.27	124.72	119.24
1	A	429	ARG	C-N-CA	5.27	124.72	119.24
1	A	171	SER	N-CA-C	5.17	116.21	108.76
1	A	557	SER	N-CA-C	5.10	116.99	108.99

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	7783	0	7721	111	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7778	0	7718	115	0
2	C	62	0	60	4	0
2	D	62	0	60	4	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	384	0	0	31	0
4	B	338	0	0	23	0
4	C	2	0	0	0	0
All	All	16411	0	15559	230	1

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 7.

All (230) 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:908:TYR:HE1	4:A:1368:HOH:O	1.18	1.23
1:A:667:MET:HG3	4:A:1031:HOH:O	1.39	1.22
1:A:908:TYR:CE1	4:A:1368:HOH:O	1.94	1.10
4:A:1311:HOH:O	2:C:17:LEU:HB3	1.53	1.08
1:B:154:SER:HB3	4:B:1351:HOH:O	1.53	1.08
1:B:736:GLN:HG2	4:B:1223:HOH:O	1.68	0.93
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.21	0.88
2:C:16:THR:HB	2:C:17:LEU:HA	1.59	0.84
1:A:243:LYS:HG3	4:A:1121:HOH:O	1.76	0.84
1:A:309:ASP:H	1:A:672:ASN:HD21	1.26	0.83
1:B:329:ASN:HD21	1:B:363:GLN:HE22	1.26	0.81
1:A:854:LYS:HD2	1:A:855:PRO:HD2	1.61	0.80
1:B:875:GLU:HG2	4:B:1312:HOH:O	1.81	0.80
1:B:309:ASP:H	1:B:672:ASN:HD21	1.29	0.79
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.64	0.78
1:B:102:ASN:HD22	1:B:102:ASN:H	1.33	0.77
1:A:491:ARG:HG2	1:A:491:ARG:HH11	1.48	0.76
2:D:17:LEU:HD13	2:D:18:GLN:HG3	1.66	0.76
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.34	0.76
1:B:134:HIS:HB3	4:B:1351:HOH:O	1.86	0.75
1:A:582:PHE:CE2	1:A:718:GLN:HG2	2.22	0.75
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.69	0.75
1:B:294:GLN:H	1:B:297:HIS:HD2	1.35	0.74
1:A:296:GLU:HG3	4:A:1335:HOH:O	1.89	0.73
1:A:107:SER:HB3	4:A:1388:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:H	1:A:102:ASN:HD22	1.37	0.72
1:A:527:LYS:HD3	4:A:1033:HOH:O	1.90	0.71
1:B:579:PHE:HE2	1:B:765:ARG:HH12	1.37	0.71
1:B:658:ARG:NH2	4:B:1118:HOH:O	2.23	0.71
1:A:619:ASP:HB2	4:A:1352:HOH:O	1.91	0.71
1:A:294:GLN:H	1:A:297:HIS:HD2	1.37	0.71
1:A:771:LEU:HD21	1:A:954:VAL:HG23	1.71	0.71
1:A:527:LYS:HE3	4:A:1115:HOH:O	1.91	0.71
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.89	0.70
1:A:316:THR:CG2	4:A:1102:HOH:O	2.40	0.70
1:A:423:ARG:HG2	1:A:423:ARG:HH11	1.55	0.69
1:B:309:ASP:H	1:B:672:ASN:ND2	1.90	0.69
1:B:782:ARG:NH1	1:B:961:ARG:O	2.25	0.69
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.75	0.68
1:B:236:ASP:CG	1:B:239:GLN:HG2	2.19	0.67
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.42	0.67
1:A:125:ASN:H	1:A:125:ASN:HD22	1.41	0.67
1:B:296:GLU:HG3	4:B:1263:HOH:O	1.95	0.67
1:B:783:ASN:ND2	1:B:785:VAL:H	1.94	0.66
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.09	0.66
1:A:316:THR:HG23	4:A:1102:HOH:O	1.96	0.66
1:A:550:LEU:HD11	1:A:558:LYS:HG3	1.78	0.65
1:A:582:PHE:CE2	1:A:718:GLN:CG	2.79	0.65
1:B:125:ASN:HD22	1:B:125:ASN:H	1.45	0.65
1:B:320:PRO:HG2	1:B:466:MET:HE1	1.78	0.64
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.97	0.64
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.27	0.63
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.95	0.63
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.80	0.63
1:B:134:HIS:HE1	4:B:1058:HOH:O	1.82	0.62
1:A:784:GLU:HB3	4:A:1269:HOH:O	2.00	0.62
1:A:783:ASN:ND2	1:A:786:HIS:H	1.98	0.61
1:A:1011:HIS:HD2	4:A:1379:HOH:O	1.83	0.61
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.18	0.61
1:A:423:ARG:HH11	1:A:423:ARG:CG	2.13	0.60
1:A:309:ASP:H	1:A:672:ASN:ND2	1.96	0.60
1:B:782:ARG:HH21	1:B:784:GLU:HG2	1.66	0.60
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.51	0.59
1:A:316:THR:HB	1:A:374:ILE:HG22	1.84	0.59
1:B:94:ILE:HB	4:B:1305:HOH:O	2.03	0.58
1:B:827:GLU:OE1	1:B:862:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TYR:OH	1:B:229:ARG:NH1	2.37	0.58
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.85	0.58
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.85	0.58
1:B:141:PHE:HB2	2:D:14:VAL:HG13	1.84	0.58
1:B:783:ASN:ND2	1:B:786:HIS:H	2.02	0.58
1:A:431:ARG:CZ	4:A:1323:HOH:O	2.51	0.58
1:B:783:ASN:HD22	1:B:785:VAL:H	1.52	0.57
1:A:491:ARG:HG2	1:A:491:ARG:NH1	2.20	0.57
1:A:927:TYR:O	1:A:930:THR:HB	2.05	0.56
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.87	0.56
1:B:622:ASN:HD22	1:B:622:ASN:H	1.54	0.56
1:A:222:ASN:O	1:A:226:LEU:HB2	2.05	0.56
1:B:451:THR:HB	1:B:455:LEU:HD12	1.88	0.56
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.35	0.56
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.40	0.55
1:A:524:LEU:HD12	4:A:1171:HOH:O	2.06	0.55
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.55	0.55
1:B:927:TYR:O	1:B:930:THR:HB	2.07	0.55
1:A:67:LEU:HD23	1:A:75:VAL:HB	1.89	0.54
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.90	0.54
1:A:879:GLU:HG2	4:B:1074:HOH:O	2.07	0.54
1:B:86:SER:HB3	1:B:158:LEU:HG	1.90	0.53
1:B:239:GLN:O	1:B:243:LYS:HG2	2.07	0.53
1:B:309:ASP:N	1:B:672:ASN:HD21	2.05	0.53
1:B:475:ASN:HB3	4:B:1218:HOH:O	2.08	0.53
1:A:483:LYS:O	1:A:486:GLU:HB2	2.08	0.53
1:B:782:ARG:NH2	1:B:784:GLU:HG2	2.22	0.53
1:A:527:LYS:CD	4:A:1033:HOH:O	2.53	0.53
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.40	0.52
1:A:529:GLU:HG3	4:A:1382:HOH:O	2.09	0.52
1:B:307:ILE:O	1:B:674:ARG:NH2	2.42	0.52
1:A:446:LEU:O	1:A:449:VAL:HG22	2.09	0.52
1:B:658:ARG:O	1:B:662:ILE:HG12	2.09	0.52
1:B:538:LEU:HD23	1:B:734:THR:HG23	1.91	0.52
1:A:466:MET:HE3	1:A:470:LYS:HE3	1.92	0.51
1:A:194:VAL:HG12	1:A:195:MET:CE	2.41	0.51
1:B:997:GLU:HG2	4:B:1039:HOH:O	2.11	0.51
1:B:597:LEU:HG	1:B:620:LEU:HG	1.93	0.50
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.93	0.50
1:B:803:SER:HA	1:B:927:TYR:CE2	2.46	0.50
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:HD2	4:A:1280:HOH:O	1.94	0.50
1:B:722:ARG:HH21	1:B:756:LYS:HD3	1.77	0.50
1:B:507:ASP:O	1:B:511:LYS:HD3	2.11	0.50
1:B:196:ASN:C	1:B:196:ASN:HD22	2.20	0.49
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.94	0.49
1:B:329:ASN:ND2	1:B:363:GLN:HE22	2.03	0.49
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.45	0.49
1:B:730:HIS:HD2	1:B:904:SER:OG	1.96	0.49
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.60	0.49
1:B:192:LYS:HD2	1:B:832:ILE:HD11	1.95	0.49
1:A:783:ASN:ND2	1:A:785:VAL:H	2.10	0.49
1:B:196:ASN:ND2	1:B:198:ALA:H	2.11	0.49
1:A:622:ASN:HD22	1:A:622:ASN:H	1.61	0.49
1:A:470:LYS:HE2	4:A:1086:HOH:O	2.13	0.49
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.93	0.49
1:A:507:ASP:O	1:A:511:LYS:HD3	2.13	0.48
1:B:616:LEU:HD21	1:B:638:GLN:HG2	1.95	0.48
1:A:658:ARG:NH2	4:A:1297:HOH:O	2.45	0.48
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.12	0.48
1:A:582:PHE:CD2	1:A:718:GLN:HG3	2.49	0.48
1:B:643:LYS:HG2	1:B:744:MET:SD	2.54	0.48
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.44	0.48
1:A:120:LYS:HE3	1:B:409:TRP:CD1	2.49	0.48
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.96	0.48
1:A:783:ASN:HD22	1:A:785:VAL:H	1.62	0.48
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.49	0.48
1:A:230:PRO:HA	1:A:235:ILE:HD12	1.95	0.47
1:B:121:TYR:HB3	1:B:126:GLU:HG2	1.95	0.47
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.48	0.47
1:B:140:ALA:HB1	4:B:1353:HOH:O	2.13	0.47
1:B:550:LEU:HD11	1:B:558:LYS:HG3	1.95	0.47
1:A:136:GLY:O	1:A:892:ARG:NH1	2.48	0.47
1:A:433:TYR:O	1:A:437:ILE:HG12	2.14	0.47
1:A:48:LYS:NZ	4:A:1363:HOH:O	2.47	0.47
1:A:793:ILE:O	1:A:847:ARG:HA	2.15	0.47
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.61	0.47
1:B:184:ASN:ND2	1:B:223:LYS:HZ1	2.12	0.46
1:A:466:MET:HE2	1:A:467:VAL:HA	1.98	0.46
1:B:444:TYR:CD1	1:B:452:ALA:HB1	2.50	0.46
1:A:102:ASN:HD22	1:A:102:ASN:N	2.08	0.46
1:B:754:HIS:CD2	4:B:1341:HOH:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASP:N	1:A:672:ASN:HD21	2.05	0.46
1:A:950:ARG:HD2	4:A:1194:HOH:O	2.15	0.46
1:B:392:LEU:HD22	1:B:512:LYS:HE2	1.98	0.46
1:B:51:GLY:O	4:B:1241:HOH:O	2.20	0.46
1:B:930:THR:HG21	4:B:1326:HOH:O	2.16	0.46
1:B:294:GLN:H	1:B:297:HIS:CD2	2.23	0.46
1:B:529:GLU:HG3	4:B:1199:HOH:O	2.15	0.46
1:B:667:MET:HE1	4:B:1052:HOH:O	2.15	0.46
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.99	0.46
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.98	0.45
1:A:730:HIS:HD2	1:A:904:SER:OG	1.99	0.45
1:A:879:GLU:HB2	4:A:1167:HOH:O	2.16	0.45
1:B:824:ARG:O	1:B:828:GLN:HA	2.17	0.45
2:C:16:THR:HB	2:C:17:LEU:CA	2.38	0.45
2:C:16:THR:CB	2:C:17:LEU:HA	2.40	0.45
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.98	0.45
1:A:618:TYR:HA	1:A:630:SER:O	2.17	0.45
1:A:862:ARG:HD2	4:A:1111:HOH:O	2.16	0.45
1:B:386:HIS:HD2	1:B:389:ASP:OD2	2.00	0.45
1:B:843:ILE:HG22	1:B:844:GLN:N	2.32	0.45
1:B:1000:ARG:NH1	4:B:1039:HOH:O	2.50	0.45
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.52	0.44
1:B:688:LEU:HD13	1:B:995:MET:HE1	1.99	0.44
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.44
1:A:239:GLN:O	1:A:243:LYS:HG2	2.17	0.44
1:A:477:ARG:HD3	4:A:1383:HOH:O	2.17	0.44
1:B:908:TYR:HE1	4:B:1316:HOH:O	2.00	0.44
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.17	0.44
1:B:722:ARG:HD2	4:B:1274:HOH:O	2.17	0.44
1:B:941:LYS:HE2	4:B:1245:HOH:O	2.16	0.44
1:B:110:LEU:HD23	1:B:110:LEU:C	2.43	0.44
1:A:599:LEU:HD21	1:A:659:PHE:HA	2.00	0.44
1:B:911:ILE:HG21	4:B:1316:HOH:O	2.18	0.44
1:A:803:SER:HA	1:A:927:TYR:CE2	2.54	0.43
1:B:843:ILE:HG22	1:B:844:GLN:H	1.83	0.43
1:A:782:ARG:HD2	4:A:1373:HOH:O	2.18	0.43
1:B:444:TYR:CE1	1:B:452:ALA:HB1	2.53	0.43
1:B:85:LYS:NZ	4:B:1238:HOH:O	2.46	0.43
1:A:156:GLU:H	1:A:156:GLU:HG2	1.66	0.43
1:A:466:MET:HE2	1:A:466:MET:C	2.44	0.43
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:OD1	1:A:589:HIS:HD2	2.02	0.43
1:B:102:ASN:HD22	1:B:102:ASN:N	2.08	0.43
1:B:433:TYR:O	1:B:437:ILE:HG12	2.19	0.43
1:B:961:ARG:HD2	1:B:962:GLU:OE1	2.19	0.43
1:A:48:LYS:HD3	4:A:1339:HOH:O	2.19	0.43
1:A:979:ASN:N	4:A:1089:HOH:O	2.52	0.42
1:A:94:ILE:HG13	1:A:248:TYR:HB3	2.01	0.42
1:B:49:ARG:HG2	1:B:68:GLU:HB3	2.01	0.42
1:A:67:LEU:HD11	1:A:268:THR:HG23	2.01	0.42
1:A:582:PHE:HE2	1:A:718:GLN:HG2	1.79	0.42
1:A:806:MET:HE3	1:A:928:LEU:HG	2.01	0.42
1:B:709:LEU:HB3	1:B:710:PRO:HD3	2.02	0.42
1:A:196:ASN:HD22	1:A:199:TRP:H	1.66	0.42
1:A:600:LEU:HD23	1:A:620:LEU:HD21	2.01	0.42
1:A:817:GLU:HB3	1:A:818:PRO:HD3	2.01	0.42
1:B:141:PHE:HB2	2:D:14:VAL:CG1	2.49	0.42
1:B:886:ILE:HG23	1:B:928:LEU:HD13	2.01	0.42
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.54	0.42
1:A:465:GLU:HB2	4:A:1168:HOH:O	2.20	0.42
1:B:112:HIS:HA	2:D:17:LEU:HD23	2.02	0.42
1:A:597:LEU:HG	1:A:620:LEU:HG	2.01	0.41
1:B:163:ASP:O	1:B:167:GLN:HG2	2.20	0.41
1:B:418:ASN:ND2	1:B:454:TYR:O	2.53	0.41
1:A:402:ARG:NH2	4:A:1190:HOH:O	2.53	0.41
1:B:908:TYR:O	1:B:912:ILE:HG12	2.21	0.41
1:A:245:HIS:O	1:A:249:TYR:HB2	2.20	0.41
1:A:329:ASN:HD21	1:A:363:GLN:HE22	1.69	0.41
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.56	0.41
1:B:389:ASP:O	1:B:393:HIS:HD2	2.04	0.41
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.74	0.41
1:B:810:LEU:HG	1:B:928:LEU:HD21	2.03	0.41
1:A:824:ARG:O	1:A:828:GLN:HA	2.20	0.40
1:A:854:LYS:CD	1:A:855:PRO:HD2	2.43	0.40
1:A:392:LEU:O	1:A:396:GLN:HG3	2.21	0.40
1:A:685:TYR:HB2	1:A:956:VAL:HG11	2.03	0.40
1:B:236:ASP:OD2	1:B:239:GLN:HG2	2.21	0.40
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.95	0.40
1:B:768:GLU:HB3	1:B:843:ILE:HG13	2.04	0.40
1:A:550:LEU:CD1	1:A:558:LYS:HG3	2.47	0.40
1:B:799:MET:HG2	1:B:843:ILE:CD1	2.51	0.40
1:B:860:GLU:OE1	1:B:953:LYS:NZ	2.54	0.40

All (1) 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:A:460:ARG:NH2	1:A:747:ASP:OD1[3_655]	2.05	0.15

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	947/990 (96%)	924 (98%)	23 (2%)	0	100	100
1	B	944/990 (95%)	925 (98%)	19 (2%)	0	100	100
2	C	5/67 (8%)	3 (60%)	2 (40%)	0	100	100
2	D	5/67 (8%)	5 (100%)	0	0	100	100
All	All	1901/2114 (90%)	1857 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	846/880 (96%)	782 (92%)	64 (8%)	12	15
1	B	846/880 (96%)	784 (93%)	62 (7%)	13	16
2	C	6/57 (10%)	5 (83%)	1 (17%)	2	2
2	D	6/57 (10%)	3 (50%)	3 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1704/1874 (91%)	1574 (92%)	130 (8%)	12	15

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	111	GLN
1	A	125	ASN
1	A	148	ASN
1	A	156	GLU
1	A	158	LEU
1	A	196	ASN
1	A	201	LEU
1	A	223	LYS
1	A	226	LEU
1	A	270	LEU
1	A	285	LEU
1	A	316	THR
1	A	329	ASN
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	414	LEU
1	A	417	LEU
1	A	423	ARG
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	491	ARG
1	A	512	LYS
1	A	558	LYS
1	A	582	PHE
1	A	595	LEU
1	A	597	LEU
1	A	612	GLU
1	A	616	LEU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	642	LEU
1	A	657	LYS
1	A	674	ARG
1	A	677	GLN
1	A	687	ARG
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	728	LEU
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	783	ASN
1	A	789	SER
1	A	810	LEU
1	A	823	LEU
1	A	838	ARG
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	889	LEU
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	993	GLN
1	A	1007	LEU
1	B	67	LEU
1	B	76	LEU
1	B	97	LEU
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	148	ASN
1	B	158	LEU
1	B	176	GLU
1	B	177	SER
1	B	196	ASN
1	B	201	LEU
1	B	226	LEU
1	B	239	GLN
1	B	243	LYS

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Mol	Chain	Res	Type
1	B	270	LEU
1	B	285	LEU
1	B	287	GLU
1	B	316	THR
1	B	329	ASN
1	B	337	LEU
1	B	347	LEU
1	B	356	VAL
1	B	414	LEU
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	488	LYS
1	B	512	LYS
1	B	524	LEU
1	B	558	LYS
1	B	595	LEU
1	B	597	LEU
1	B	612	GLU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	648	LYS
1	B	657	LYS
1	B	674	ARG
1	B	677	GLN
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE
1	B	736	GLN
1	B	758	LEU
1	B	759	LEU
1	B	771	LEU
1	B	783	ASN
1	B	810	LEU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
1	B	889	LEU

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Mol	Chain	Res	Type
1	B	928	LEU
1	B	931	LEU
1	B	942	GLU
1	B	993	GLN
1	B	1007	LEU
2	C	17	LEU
2	D	14	VAL
2	D	16	THR
2	D	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	148	ASN
1	A	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS
1	A	300	GLN
1	A	329	ASN
1	A	376	ASN
1	A	393	HIS
1	A	399	GLN
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	573	ASN
1	A	575	ASN
1	A	589	HIS
1	A	622	ASN
1	A	672	ASN
1	A	718	GLN
1	A	730	HIS
1	A	770	GLN
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN

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Mol	Chain	Res	Type
1	A	922	ASN
1	A	957	HIS
1	A	982	GLN
1	B	52	ASN
1	B	93	HIS
1	B	102	ASN
1	B	125	ASN
1	B	148	ASN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	232	GLN
1	B	297	HIS
1	B	329	ASN
1	B	376	ASN
1	B	386	HIS
1	B	393	HIS
1	B	515	ASN
1	B	575	ASN
1	B	589	HIS
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	752	HIS
1	B	770	GLN
1	B	783	ASN
1	B	805	ASN
1	B	821	ASN
1	B	828	GLN
1	B	883	GLN
1	B	914	GLN
1	B	917	ASN
1	B	922	ASN
1	B	957	HIS
1	B	979	ASN
1	B	982	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	953/990 (96%)	-0.01	12 (1%) 75 76	20, 32, 47, 62	0
1	B	952/990 (96%)	0.18	26 (2%) 56 58	25, 37, 50, 71	0
2	C	9/67 (13%)	4.15	8 (88%) 0 0	37, 66, 67, 67	0
2	D	9/67 (13%)	4.01	8 (88%) 0 0	36, 73, 75, 75	0
All	All	1923/2114 (90%)	0.12	54 (2%) 55 56	20, 35, 49, 75	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	17	LEU	8.0
2	C	16	THR	6.8
2	D	16	THR	6.7
2	C	13	LEU	5.5
2	D	13	LEU	5.4
2	D	14	VAL	5.3
2	D	17	LEU	5.0
1	B	52	ASN	4.6
2	C	18	GLN	4.5
1	B	452	ALA	4.0
2	D	18	GLN	4.0
1	B	53	HIS	4.0
1	B	880	GLU	3.9
1	B	229	ARG	3.9
1	B	239	GLN	3.7
1	B	1010	PRO	3.5
1	B	979	ASN	3.5
1	A	764	VAL	3.3
1	B	1011	HIS	3.3
1	A	763	LEU	3.2
2	C	3	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	14	VAL	3.2
1	B	736	GLN	3.2
1	A	667	MET	3.1
1	B	702	GLU	3.1
1	A	43	ASN	3.1
1	B	582	PHE	2.9
2	C	15	ASP	2.9
1	B	764	VAL	2.9
1	A	1011	HIS	2.8
2	D	15	ASP	2.8
1	B	667	MET	2.8
1	B	47	ILE	2.7
1	B	1008	VAL	2.7
2	D	2	TYR	2.6
1	A	543	GLU	2.5
1	B	232	GLN	2.5
1	B	49	ARG	2.5
1	B	706	ASP	2.4
1	A	625	TYR	2.4
1	A	979	ASN	2.4
1	A	784	GLU	2.3
2	D	3	ARG	2.3
1	B	282	ASN	2.2
1	B	508	GLU	2.2
1	B	625	TYR	2.2
2	C	2	TYR	2.2
1	A	765	ARG	2.2
1	B	455	LEU	2.2
1	A	508	GLU	2.2
1	B	766	TYR	2.1
1	B	511	LYS	2.0
1	A	475	ASN	2.0
1	B	765	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	2	1/1	0.99	0.42	2,2,2,2	0
3	ZN	C	68	1/1	1.00	0.40	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.