



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:17 PM UTC

PDB ID : 4RAL / pdb_00004ral
Title : Crystal structure of insulin degrading enzyme in complex with macrophage inflammatory protein 1 beta
Authors : Liang, W.G.; Ren, M.; Guo, Q.; Tang, W.J.
Deposited on : 2014-09-10
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

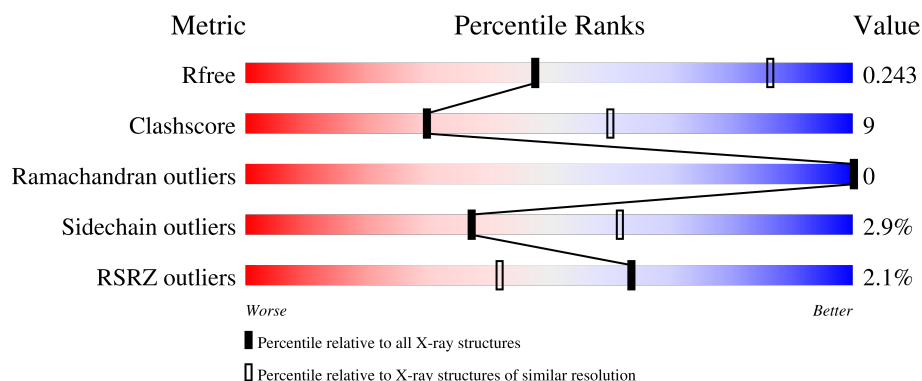
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	75% 20% ..
1	B	990	2% 73% 21% ..
2	D	69	6% 7% 9% 84%
2	E	69	6% 12% .. 86%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15826 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	954	Total	C	N	O	S	0	0	0
			7799	5024	1311	1442	22			
1	B	953	Total	C	N	O	S	0	0	0
			7790	5019	1309	1440	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called C-C motif chemokine 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total 86	C 54	N 17	O 14	S 1	0	0	0
2	E	10	Total 82	C 52	N 16	O 13	S 1	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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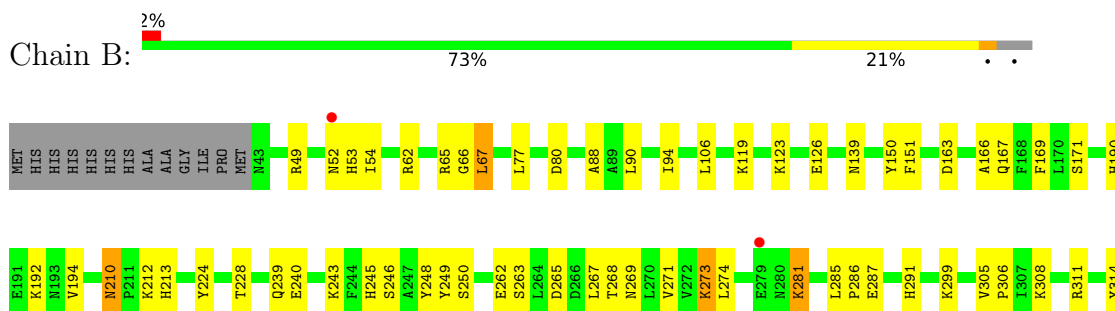
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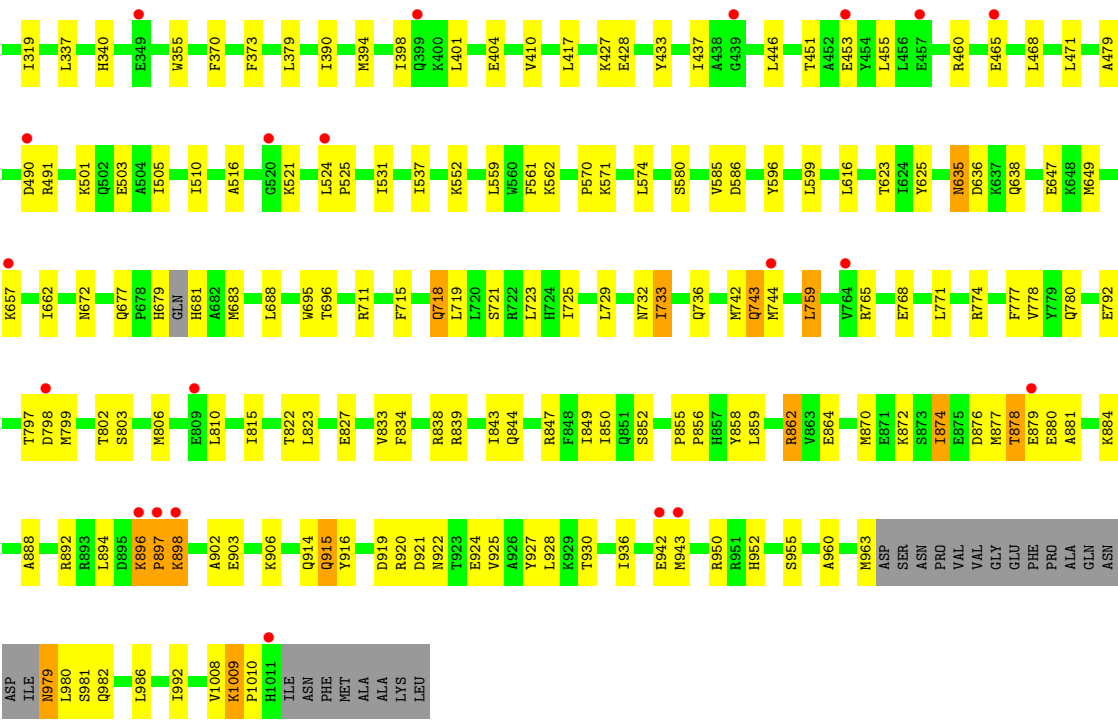
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

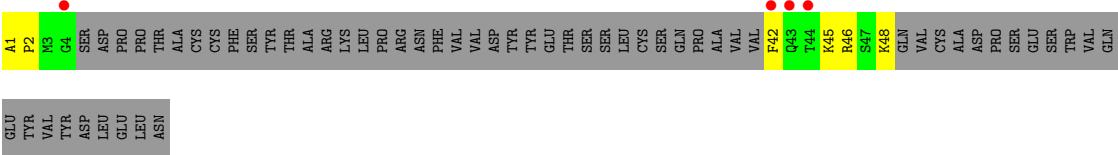
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total 41	O 41	0	0
4	B	25	Total 25	O 25	0	0
4	E	1	Total 1	O 1	0	0

- Molecule 1: Insulin-degrading enzyme

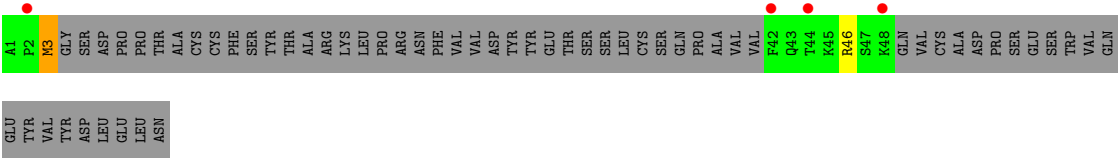




● Molecule 2: C-C motif chemokine 4



● Molecule 2: C-C motif chemokine 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	263.12Å 263.12Å 90.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.26 – 3.15 48.26 – 3.15	Depositor EDS
% Data completeness (in resolution range)	60.0 (48.26-3.15) 92.0 (48.26-3.15)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.255 0.193 , 0.243	Depositor DCC
R_{free} test set	704 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15826	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/7994	0.79	14/10815 (0.1%)
1	B	0.34	0/7984	0.82	17/10800 (0.2%)
2	D	0.38	0/86	0.79	0/110
2	E	0.25	0/82	0.71	0/105
All	All	0.33	0/16146	0.80	31/21830 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	897	PRO	N-CA-C	8.27	124.52	111.38
1	A	636	ASP	N-CA-C	7.28	119.84	111.11
1	B	759	LEU	CA-C-N	7.24	127.57	119.32
1	B	759	LEU	C-N-CA	7.24	127.57	119.32
1	B	636	ASP	N-CA-C	7.08	118.69	110.97
1	A	454	TYR	N-CA-C	7.08	121.97	113.12
1	B	879	GLU	N-CA-C	-6.73	104.93	113.01
1	A	213	HIS	N-CA-C	-6.25	102.19	110.07
1	B	915	GLN	N-CA-C	-6.24	105.80	113.41
1	A	383	GLY	N-CA-C	-6.08	107.11	114.66
1	B	898	LYS	N-CA-CB	-5.98	101.07	110.46
1	B	281	LYS	N-CA-C	-5.94	100.16	109.25
1	A	429	ARG	CA-C-N	5.88	125.35	119.24
1	A	429	ARG	C-N-CA	5.88	125.35	119.24
1	A	121	TYR	CA-C-N	5.55	125.17	119.56
1	A	121	TYR	C-N-CA	5.55	125.17	119.56
1	A	658	ARG	N-CA-C	-5.50	106.41	113.23
1	B	460	ARG	CA-C-N	5.50	125.33	119.28
1	B	460	ARG	C-N-CA	5.50	125.33	119.28
1	A	637	LYS	N-CA-C	-5.45	105.86	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	ALA	CB-CA-C	5.43	118.72	109.75
1	B	1009	LYS	CA-C-N	5.37	125.35	120.03
1	B	1009	LYS	C-N-CA	5.37	125.35	120.03
1	A	169	PHE	CB-CA-C	5.34	119.02	109.29
1	B	571	LYS	N-CA-C	5.24	117.62	110.55
1	A	500	TYR	N-CA-C	5.23	115.14	108.24
1	A	170	LEU	N-CA-C	5.22	119.55	111.56
1	B	878	THR	N-CA-C	-5.20	102.70	110.23
1	B	210	ASN	CA-C-N	5.03	124.81	119.28
1	B	210	ASN	C-N-CA	5.03	124.81	119.28
1	A	412	GLN	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7799	0	7736	128	0
1	B	7790	0	7727	140	0
2	D	86	0	93	9	0
2	E	82	0	90	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	41	0	0	3	0
4	B	25	0	0	0	0
4	E	1	0	0	0	0
All	All	15826	0	15646	268	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 9.

All (268) 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:412:GLN:HE21	1:A:412:GLN:HA	1.33	0.93
1:B:896:LYS:HB3	1:B:897:PRO:HD2	1.59	0.83
1:B:798:ASP:OD1	1:B:799:MET:N	2.15	0.79
1:A:858:TYR:CZ	1:A:862:ARG:HD2	2.17	0.79
1:B:881:ALA:HA	1:B:884:LYS:HZ2	1.49	0.76
1:B:880:GLU:HG2	1:B:884:LYS:HE3	1.68	0.73
1:B:870:MET:O	1:B:874:ILE:HG22	1.89	0.72
1:A:743:GLN:NE2	1:A:747:ASP:OD1	2.23	0.71
1:B:65:ARG:NH1	1:B:265:ASP:OD1	2.23	0.70
1:A:179:LYS:HD2	1:A:237:VAL:HB	1.74	0.70
1:B:239:GLN:N	1:B:239:GLN:OE1	2.24	0.70
1:B:896:LYS:CB	1:B:897:PRO:HD2	2.21	0.70
1:A:418:ASN:HB3	1:A:454:TYR:O	1.93	0.68
1:A:948:ALA:HB3	1:A:951:ARG:HB2	1.75	0.68
1:B:240:GLU:HA	1:B:243:LYS:HG2	1.76	0.67
1:A:424:PHE:O	1:A:571:LYS:NZ	2.28	0.66
1:B:896:LYS:HB3	1:B:897:PRO:CD	2.26	0.66
1:B:623:THR:HG23	1:B:625:TYR:H	1.60	0.66
1:B:427:LYS:HG2	1:B:898:LYS:HD3	1.78	0.65
1:A:596:TYR:CD1	1:A:716:ILE:HG12	2.31	0.65
1:B:246:SER:OG	1:B:281:LYS:NZ	2.30	0.65
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.79	0.65
1:B:858:TYR:CZ	1:B:862:ARG:HD2	2.33	0.64
1:B:67:LEU:HD21	1:B:268:THR:HG23	1.79	0.64
1:B:269:ASN:HB3	1:B:273:LYS:HZ1	1.62	0.64
1:B:896:LYS:CB	1:B:897:PRO:CD	2.75	0.64
1:B:765:ARG:CZ	1:B:914:GLN:HE22	2.10	0.64
1:A:862:ARG:CZ	1:A:862:ARG:HA	2.27	0.63
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.81	0.62
1:B:799:MET:HE3	1:B:1008:VAL:HG22	1.82	0.62
1:B:896:LYS:HE2	1:B:921:ASP:OD2	2.00	0.61
1:A:491:ARG:NH2	1:A:500:TYR:OH	2.33	0.61
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.82	0.61
1:B:715:PHE:CZ	1:B:719:LEU:HD22	2.35	0.61
1:B:570:PRO:O	1:B:635:ASN:ND2	2.33	0.61
1:A:210:ASN:HB3	1:A:213:HIS:HB2	1.81	0.61
1:A:858:TYR:CE2	1:A:862:ARG:HD2	2.36	0.61
1:B:919:ASP:OD1	1:B:922:ASN:ND2	2.34	0.61
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.82	0.60
1:B:427:LYS:HB3	1:B:898:LYS:HG2	1.84	0.60
1:B:490:ASP:OD1	1:B:491:ARG:NH1	2.35	0.60
1:A:858:TYR:O	1:A:862:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:ILE:HG22	1:B:870:MET:HE2	1.84	0.59
1:A:285:LEU:HD22	1:A:286:PRO:HD2	1.83	0.59
1:A:491:ARG:HG2	1:A:492:THR:H	1.68	0.59
1:A:768:GLU:HB3	1:A:843:ILE:HD13	1.85	0.59
1:B:768:GLU:HB3	1:B:843:ILE:HD13	1.84	0.58
1:B:337:LEU:HD11	1:B:410:VAL:HG11	1.85	0.58
1:A:697:LYS:O	1:A:701:LYS:HG3	2.04	0.58
1:B:797:THR:HG22	1:B:943:MET:HG3	1.86	0.57
1:A:252:ASN:ND2	1:A:283:VAL:O	2.36	0.57
1:A:831:TYR:HE2	2:D:48:LYS:HD3	1.69	0.57
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.86	0.57
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.87	0.57
1:B:679:HIS:O	1:B:681:HIS:N	2.39	0.56
1:A:412:GLN:HA	1:A:412:GLN:NE2	2.13	0.56
1:B:210:ASN:HB3	1:B:213:HIS:HB2	1.88	0.56
1:B:250:SER:OG	1:B:281:LYS:O	2.21	0.55
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.87	0.55
1:A:43:ASN:OD1	1:A:44:ASN:N	2.40	0.55
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.89	0.55
1:B:778:VAL:HG22	1:B:955:SER:HB2	1.89	0.55
1:B:896:LYS:HZ1	1:B:906:LYS:HD2	1.72	0.54
1:A:295:GLU:N	1:A:295:GLU:OE1	2.40	0.54
1:A:192:LYS:HE3	2:D:48:LYS:HE3	1.88	0.54
1:A:794:TYR:CE1	1:A:838:ARG:HD3	2.43	0.54
1:B:942:GLU:OE1	1:B:943:MET:HG2	2.07	0.54
1:A:776:TRP:CD2	1:A:989:PRO:HB3	2.43	0.54
1:B:524:LEU:HG	1:B:525:PRO:HD2	1.89	0.54
1:A:671:ASN:OD1	1:A:701:LYS:HD2	2.08	0.53
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.90	0.53
1:B:299:LYS:HD2	1:B:510:ILE:HD13	1.90	0.53
1:A:412:GLN:HE21	1:A:412:GLN:CA	2.10	0.53
1:A:192:LYS:HE3	2:D:48:LYS:CE	2.38	0.53
1:A:253:LEU:HD22	1:A:285:LEU:HD23	1.91	0.53
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.91	0.53
1:B:950:ARG:O	1:B:952:HIS:CE1	2.62	0.53
1:A:778:VAL:HG22	1:A:955:SER:HB2	1.91	0.53
1:B:798:ASP:CG	1:B:799:MET:H	2.15	0.53
1:B:62:ARG:HG2	1:B:80:ASP:HB2	1.92	0.52
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.90	0.52
1:A:361:GLY:O	2:D:2:PRO:HA	2.09	0.52
1:B:802:THR:HG23	1:B:924:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:NH2	4:A:1217:HOH:O	2.43	0.52
1:A:847:ARG:NH1	4:A:1215:HOH:O	2.38	0.52
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.92	0.52
1:B:570:PRO:O	1:B:635:ASN:CG	2.53	0.52
1:A:864:GLU:HG3	1:A:986:LEU:HD11	1.91	0.51
1:B:224:TYR:HA	1:B:228:THR:HB	1.91	0.51
1:B:340:HIS:CE1	1:B:525:PRO:HB3	2.46	0.51
1:B:822:THR:O	1:B:827:GLU:HG3	2.11	0.51
1:A:834:PHE:HB3	1:A:849:ILE:HB	1.92	0.51
1:A:311:ARG:HD3	1:A:384:LEU:HD22	1.92	0.51
1:A:870:MET:O	1:A:874:ILE:HG12	2.11	0.51
1:A:141:PHE:HB3	2:D:45:LYS:HG2	1.92	0.51
1:B:314:TYR:HB2	1:B:479:ALA:HB3	1.92	0.51
1:A:189:GLU:O	1:A:192:LYS:HG2	2.11	0.51
1:A:245:HIS:O	1:A:249:TYR:HB2	2.11	0.51
1:B:192:LYS:HG3	1:B:677:GLN:OE1	2.10	0.51
1:A:950:ARG:O	1:A:952:HIS:CE1	2.63	0.51
1:B:765:ARG:NE	1:B:914:GLN:HE22	2.09	0.50
1:A:596:TYR:OH	1:A:649:MET:O	2.28	0.50
1:A:765:ARG:HD3	1:A:914:GLN:HG3	1.93	0.50
1:A:460:ARG:NH1	1:A:462:ASP:OD2	2.44	0.50
1:A:852:SER:HB3	1:A:859:LEU:HD11	1.91	0.50
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.93	0.50
1:A:192:LYS:HE2	1:A:193:ASN:OD1	2.12	0.50
1:B:915:GLN:OE1	1:B:920:ARG:NH2	2.43	0.50
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.47	0.50
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.93	0.50
1:B:725:ILE:HG21	1:B:742:MET:HE1	1.94	0.49
1:B:311:ARG:NH1	1:B:379:LEU:O	2.44	0.49
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.95	0.49
1:A:743:GLN:HE21	1:A:747:ASP:CG	2.21	0.49
1:B:49:ARG:HH21	1:B:446:LEU:HD23	1.77	0.49
1:A:725:ILE:HG21	1:A:742:MET:HE1	1.94	0.49
1:B:262:GLU:HB2	1:B:267:LEU:HD13	1.95	0.49
1:B:839:ARG:NH1	1:B:844:GLN:OE1	2.46	0.49
1:A:886:ILE:HG23	1:A:928:LEU:HG	1.94	0.49
1:A:192:LYS:HB2	1:A:677:GLN:OE1	2.13	0.49
1:A:198:ALA:HB1	2:D:42:PHE:CZ	2.48	0.49
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.93	0.49
1:B:505:ILE:HB	1:B:510:ILE:HD11	1.94	0.48
1:A:49:ARG:HG2	1:A:68:GLU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD12	1:B:471:LEU:HD12	1.96	0.48
1:B:88:ALA:HB3	1:B:151:PHE:CE1	2.48	0.48
1:B:823:LEU:HD13	1:B:850:ILE:HD11	1.95	0.48
1:A:751:GLU:OE1	1:A:752:HIS:ND1	2.46	0.48
1:B:688:LEU:HD13	1:B:696:THR:HG22	1.95	0.48
1:B:119:LYS:HE2	1:B:171:SER:HB3	1.95	0.48
1:B:715:PHE:CE2	1:B:719:LEU:HD22	2.49	0.48
1:A:875:GLU:HB3	1:B:53:HIS:HE1	1.79	0.48
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.47	0.48
1:B:979:ASN:N	1:B:979:ASN:ND2	2.60	0.48
1:B:537:ILE:HA	1:B:732:ASN:HD21	1.79	0.47
1:A:150:TYR:HE1	1:A:431:ARG:HE	1.61	0.47
1:B:914:GLN:HG2	1:B:916:TYR:OH	2.14	0.47
1:A:201:LEU:HD21	1:A:481:VAL:HG21	1.97	0.47
1:B:66:GLY:C	1:B:67:LEU:HD12	2.40	0.47
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.96	0.47
1:B:777:PHE:HB3	1:B:992:ILE:HD11	1.97	0.47
1:B:922:ASN:ND2	1:B:922:ASN:H	2.13	0.47
1:A:667:MET:HE2	1:A:704:LEU:HD23	1.97	0.47
1:A:959:LEU:HB3	1:A:963:MET:HG3	1.97	0.47
1:A:1009:LYS:HA	1:A:1010:PRO:HD3	1.74	0.47
1:B:942:GLU:CD	1:B:943:MET:HG2	2.40	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.50	0.46
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.98	0.46
1:A:746:GLU:O	1:A:750:ILE:HG13	2.16	0.46
1:B:834:PHE:HB3	1:B:849:ILE:HB	1.97	0.46
1:B:269:ASN:HB3	1:B:273:LYS:NZ	2.28	0.46
1:B:896:LYS:CG	1:B:897:PRO:HD2	2.46	0.46
1:B:106:LEU:HD21	1:B:240:GLU:O	2.16	0.46
1:B:428:GLU:HG3	1:B:433:TYR:CE1	2.51	0.46
1:A:47:ILE:HG21	1:A:50:ILE:HD11	1.98	0.46
1:B:166:ALA:HB3	1:B:274:LEU:HD22	1.97	0.46
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.98	0.45
1:B:355:TRP:HB3	1:B:390:ILE:HD11	1.98	0.45
1:A:200:ARG:NH2	4:A:1237:HOH:O	2.49	0.45
1:A:674:ARG:NH1	1:A:784:GLU:OE2	2.49	0.45
1:B:501:LYS:NZ	1:B:503:GLU:OE1	2.46	0.45
1:B:743:GLN:HE21	1:B:743:GLN:HB3	1.58	0.45
1:A:810:LEU:HD23	1:A:936:ILE:HD11	1.98	0.45
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.97	0.45
1:A:311:ARG:NH1	1:A:379:LEU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:THR:HA	1:A:943:MET:HE2	1.98	0.45
1:A:915:GLN:OE1	1:A:920:ARG:NH2	2.48	0.45
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.64	0.45
1:B:245:HIS:O	1:B:249:TYR:HB2	2.16	0.45
1:B:838:ARG:HB2	1:B:847:ARG:HD3	1.99	0.45
1:B:190:HIS:O	1:B:194:VAL:HG23	2.17	0.45
1:B:337:LEU:HD23	1:B:401:LEU:HD22	1.98	0.45
1:B:888:ALA:O	1:B:892:ARG:HG3	2.17	0.45
1:A:807:PHE:HE1	1:A:931:LEU:HG	1.82	0.45
1:A:437:ILE:HA	1:A:440:ILE:HG12	1.98	0.45
1:A:305:VAL:HA	1:A:306:PRO:HD3	1.86	0.45
1:B:433:TYR:CE1	1:B:437:ILE:HD11	2.52	0.44
1:A:994:ASN:HB3	1:A:997:GLU:HB3	1.98	0.44
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.53	0.44
1:B:765:ARG:NH2	1:B:914:GLN:HE22	2.14	0.44
1:B:852:SER:HB3	1:B:859:LEU:HD11	1.99	0.44
1:B:878:THR:C	1:B:880:GLU:N	2.73	0.44
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.75	0.44
1:A:163:ASP:HA	1:A:274:LEU:HD13	1.99	0.44
1:A:460:ARG:O	1:A:464:ILE:HG12	2.18	0.44
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.99	0.44
1:B:878:THR:O	1:B:881:ALA:N	2.49	0.44
1:B:896:LYS:HZ1	1:B:906:LYS:CD	2.30	0.44
1:A:831:TYR:CE2	2:D:48:LYS:HD3	2.51	0.44
1:A:170:LEU:HD13	1:A:277:GLU:OE1	2.17	0.44
1:A:355:TRP:HB3	1:A:390:ILE:HD11	1.99	0.44
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.99	0.44
1:B:862:ARG:HA	1:B:862:ARG:CZ	2.47	0.44
1:A:111:GLN:HE21	2:D:46:ARG:HB2	1.83	0.44
1:B:427:LYS:HD3	1:B:898:LYS:CG	2.48	0.43
1:A:556:MET:HE1	1:A:756:LYS:HA	2.01	0.43
1:B:596:TYR:OH	1:B:649:MET:O	2.34	0.43
1:B:561:PHE:HE1	1:B:733:ILE:HD12	1.84	0.43
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.99	0.43
1:A:80:ASP:OD1	1:A:82:THR:HG22	2.18	0.43
1:A:701:LYS:HB2	1:A:701:LYS:HE2	1.70	0.43
1:B:897:PRO:HB3	1:B:902:ALA:HB3	1.99	0.43
1:A:948:ALA:HA	1:A:949:PRO:HD3	1.80	0.43
1:B:616:LEU:HD11	1:B:638:GLN:HG3	2.00	0.43
1:A:109:PHE:CZ	1:A:183:VAL:HG23	2.54	0.43
1:A:321:ASP:HA	1:A:371:MET:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:HA3	1:A:363:GLN:OE1	2.18	0.43
1:A:429:ARG:H	1:A:429:ARG:HG3	1.51	0.43
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.54	0.42
1:B:880:GLU:HG2	1:B:884:LYS:CE	2.42	0.42
1:A:308:LYS:HD3	1:A:672:ASN:HB3	2.00	0.42
1:A:491:ARG:HG2	1:A:492:THR:N	2.33	0.42
1:A:349:GLU:OE1	1:A:521:LYS:HE3	2.19	0.42
1:A:191:GLU:O	1:A:194:VAL:HG12	2.19	0.42
1:B:896:LYS:HG3	1:B:897:PRO:CD	2.50	0.42
1:A:817:GLU:HB3	1:A:818:PRO:HD3	2.02	0.42
1:B:562:LYS:NZ	1:B:903:GLU:OE1	2.40	0.42
1:B:163:ASP:O	1:B:167:GLN:HG2	2.19	0.42
1:B:319:ILE:HD13	1:B:373:PHE:HB2	2.02	0.42
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.95	0.42
1:B:858:TYR:CE2	1:B:862:ARG:HD2	2.54	0.42
1:B:823:LEU:HB2	1:B:833:VAL:HG11	2.02	0.42
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.55	0.42
1:A:339:GLY:O	2:D:1:ALA:N	2.49	0.42
1:A:773:ASP:HB3	1:A:949:PRO:O	2.20	0.42
1:A:586:ASP:OD1	1:A:589:HIS:ND1	2.53	0.42
1:A:736:GLN:H	1:A:736:GLN:HG3	1.51	0.42
1:B:559:LEU:HD11	1:B:729:LEU:HG	2.01	0.42
1:B:285:LEU:HD12	1:B:286:PRO:HD2	2.03	0.41
1:B:417:LEU:HD13	1:B:531:ILE:HD12	2.01	0.41
1:B:465:GLU:HA	1:B:468:LEU:HB3	2.02	0.41
1:B:803:SER:HA	1:B:927:TYR:CE2	2.55	0.41
1:B:1009:LYS:HA	1:B:1010:PRO:HD3	1.72	0.41
1:A:798:ASP:OD1	1:A:799:MET:N	2.32	0.41
1:B:54:ILE:HD11	1:B:66:GLY:H	1.85	0.41
1:A:534:ASN:OD1	1:A:536:GLU:HG3	2.20	0.41
1:A:716:ILE:HB	1:A:717:PRO:HD3	2.02	0.41
1:A:862:ARG:HA	1:A:862:ARG:NH1	2.35	0.41
1:B:49:ARG:NH2	1:B:446:LEU:HD23	2.35	0.41
1:B:139:ASN:OD1	2:E:46:ARG:HB3	2.19	0.41
1:B:806:MET:HE2	1:B:928:LEU:HB2	2.02	0.41
1:A:934:GLU:O	1:A:938:LYS:HG3	2.21	0.41
1:B:683:MET:HA	1:B:792:GLU:OE2	2.21	0.41
1:B:864:GLU:HG3	1:B:986:LEU:HD11	2.03	0.41
1:B:927:TYR:O	1:B:930:THR:OG1	2.34	0.41
1:A:570:PRO:O	1:A:635:ASN:CG	2.64	0.41
2:E:3:MET:HB3	2:E:3:MET:HE2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HD3	1:A:424:PHE:CZ	2.56	0.41
1:A:596:TYR:CE1	1:A:716:ILE:CG2	3.04	0.41
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.56	0.41
1:B:263:SER:O	1:B:267:LEU:N	2.47	0.41
1:B:394:MET:O	1:B:398:ILE:HG13	2.20	0.41
1:B:718:GLN:HA	1:B:721:SER:OG	2.21	0.41
1:B:77:LEU:HD21	1:B:271:VAL:HG21	2.02	0.41
1:B:896:LYS:NZ	1:B:906:LYS:HD2	2.35	0.41
1:A:298:LEU:HD13	1:A:475:ASN:HB2	2.03	0.40
1:B:139:ASN:HB3	1:B:150:TYR:CZ	2.56	0.40
1:A:596:TYR:CE1	1:A:716:ILE:HG23	2.55	0.40
1:B:305:VAL:HA	1:B:306:PRO:HD3	1.89	0.40
1:A:80:ASP:O	1:A:83:THR:HG22	2.22	0.40
1:A:314:TYR:HB2	1:A:479:ALA:HB3	2.03	0.40
1:A:88:ALA:HB3	1:A:151:PHE:CE2	2.57	0.40
1:A:803:SER:HA	1:A:927:TYR:CE2	2.56	0.40
1:A:868:ILE:O	1:A:872:LYS:HG2	2.21	0.40
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.91	0.40
1:B:451:THR:HB	1:B:455:LEU:HD12	2.04	0.40
1:B:586:ASP:HA	1:B:695:TRP:CZ2	2.57	0.40
1:B:625:TYR:OH	1:B:765:ARG:HB3	2.22	0.40

There are no symmetry-related clashes.

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	950/990 (96%)	936 (98%)	14 (2%)	0	100	100
1	B	947/990 (96%)	929 (98%)	18 (2%)	0	100	100
2	D	7/69 (10%)	7 (100%)	0	0	100	100
2	E	6/69 (9%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1910/2118 (90%)	1878 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	848/879 (96%)	830 (98%)	18 (2%)	47	67
1	B	847/879 (96%)	816 (96%)	31 (4%)	30	57
2	D	9/63 (14%)	9 (100%)	0	100	100
2	E	9/63 (14%)	8 (89%)	1 (11%)	6	21
All	All	1713/1884 (91%)	1663 (97%)	50 (3%)	37	61

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLU
1	A	180	ASP
1	A	183	VAL
1	A	212	LYS
1	A	365	GLU
1	A	412	GLN
1	A	465	GLU
1	A	494	GLU
1	A	507	ASP
1	A	517	ASP
1	A	598	GLU
1	A	701	LYS
1	A	736	GLN
1	A	853	GLU
1	A	862	ARG
1	A	898	LYS
1	A	906	LYS

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Mol	Chain	Res	Type
1	A	982	GLN
1	B	52	ASN
1	B	67	LEU
1	B	212	LYS
1	B	273	LYS
1	B	287	GLU
1	B	404	GLU
1	B	453	GLU
1	B	521	LYS
1	B	585	VAL
1	B	635	ASN
1	B	647	GLU
1	B	657	LYS
1	B	711	ARG
1	B	718	GLN
1	B	733	ILE
1	B	736	GLN
1	B	743	GLN
1	B	744	MET
1	B	759	LEU
1	B	774	ARG
1	B	780	GLN
1	B	862	ARG
1	B	872	LYS
1	B	874	ILE
1	B	876	ASP
1	B	877	MET
1	B	896	LYS
1	B	979	ASN
1	B	980	LEU
1	B	981	SER
1	B	982	GLN
2	E	3	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	515	ASN
1	A	573	ASN
1	A	605	ASN
1	A	821	ASN

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Mol	Chain	Res	Type
1	A	857	HIS
1	A	887	GLN
1	B	53	HIS
1	B	294	GLN
1	B	323	GLN
1	B	376	ASN
1	B	724	HIS
1	B	743	GLN
1	B	752	HIS
1	B	788	ASN
1	B	805	ASN
1	B	914	GLN
1	B	922	ASN

5.3.3 RNA [i](#)

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	954/990 (96%)	-0.11	10 (1%) 79 61	30, 44, 72, 116	0
1	B	953/990 (96%)	0.01	23 (2%) 59 38	32, 51, 83, 128	0
2	D	11/69 (15%)	1.68	4 (36%) 1 0	43, 74, 98, 112	0
2	E	10/69 (14%)	1.76	4 (40%) 1 0	53, 82, 99, 102	0
All	All	1928/2118 (91%)	-0.03	41 (2%) 63 42	30, 48, 80, 128	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	898	LYS	5.9
1	A	1011	HIS	4.9
1	B	520	GLY	4.2
1	B	764	VAL	3.9
2	E	48	LYS	3.7
1	B	896	LYS	3.7
1	A	212	LYS	3.4
1	A	274	LEU	3.3
1	B	943	MET	3.1
1	B	349	GLU	3.0
1	B	798	ASP	2.9
1	B	897	PRO	2.9
2	D	43	GLN	2.8
1	A	947	ASP	2.8
1	B	52	ASN	2.8
2	E	42	PHE	2.8
1	A	51	GLY	2.7
1	B	1011	HIS	2.7
1	B	465	GLU	2.6
1	B	744	MET	2.6
1	B	457	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	439	GLY	2.5
1	A	494	GLU	2.4
1	A	898	LYS	2.4
1	A	887	GLN	2.4
1	B	942	GLU	2.4
2	E	2	PRO	2.4
1	B	279	GLU	2.2
1	A	657	LYS	2.2
1	B	879	GLU	2.2
1	B	657	LYS	2.2
1	B	524	LEU	2.2
1	B	453	GLU	2.1
1	B	399	GLN	2.1
1	A	243	LYS	2.1
1	B	490	ASP	2.1
2	D	42	PHE	2.1
1	B	809	GLU	2.1
2	E	44	THR	2.0
2	D	44	THR	2.0
2	D	4	GLY	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	A	1101	1/1	0.98	0.07	71,71,71,71	0
3	ZN	B	1101	1/1	0.99	0.05	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.