



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:48 PM EDT

PDB ID : 3E50 / pdb_00003e50
Title : Crystal structure of human insulin degrading enzyme in complex with transforming growth factor- α
Authors : Guo, Q.; Manolopoulou, M.; Tang, W.-J.
Deposited on : 2008-08-12
Resolution : 2.30 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:

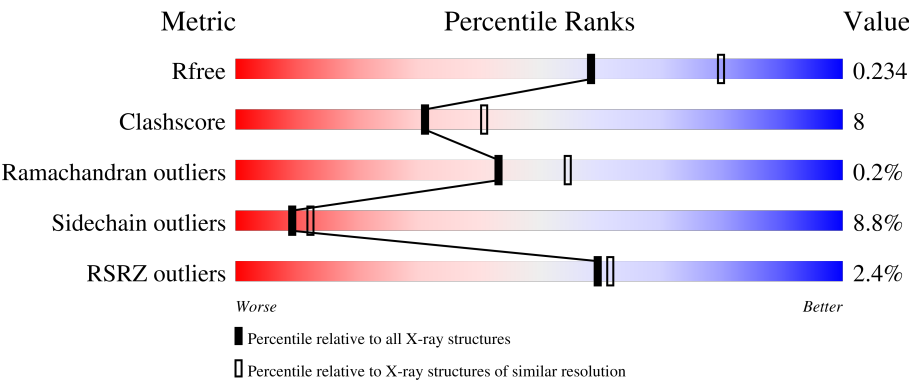
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 75% 18%
1	B	990	2% 74% 19%
2	C	50	4% 6% 90%
2	D	50	14% 12% 8% 80%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16297 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	961	Total	C	N	O	S	0	0	0
			7840	5042	1317	1447	34			
1	B	955	Total	C	N	O	S	0	0	0
			7771	4996	1306	1435	34			

There are 26 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	111	GLN	GLU	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	GLN	GLU	engineered mutation	UNP P14735

- Molecule 2 is a protein called Protransforming growth factor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			35	22	7	6			
2	D	10	Total	C	N	O	0	0	0
			81	50	15	16			

- 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		
3	D	1	Total	Zn	0	0
			1	1		

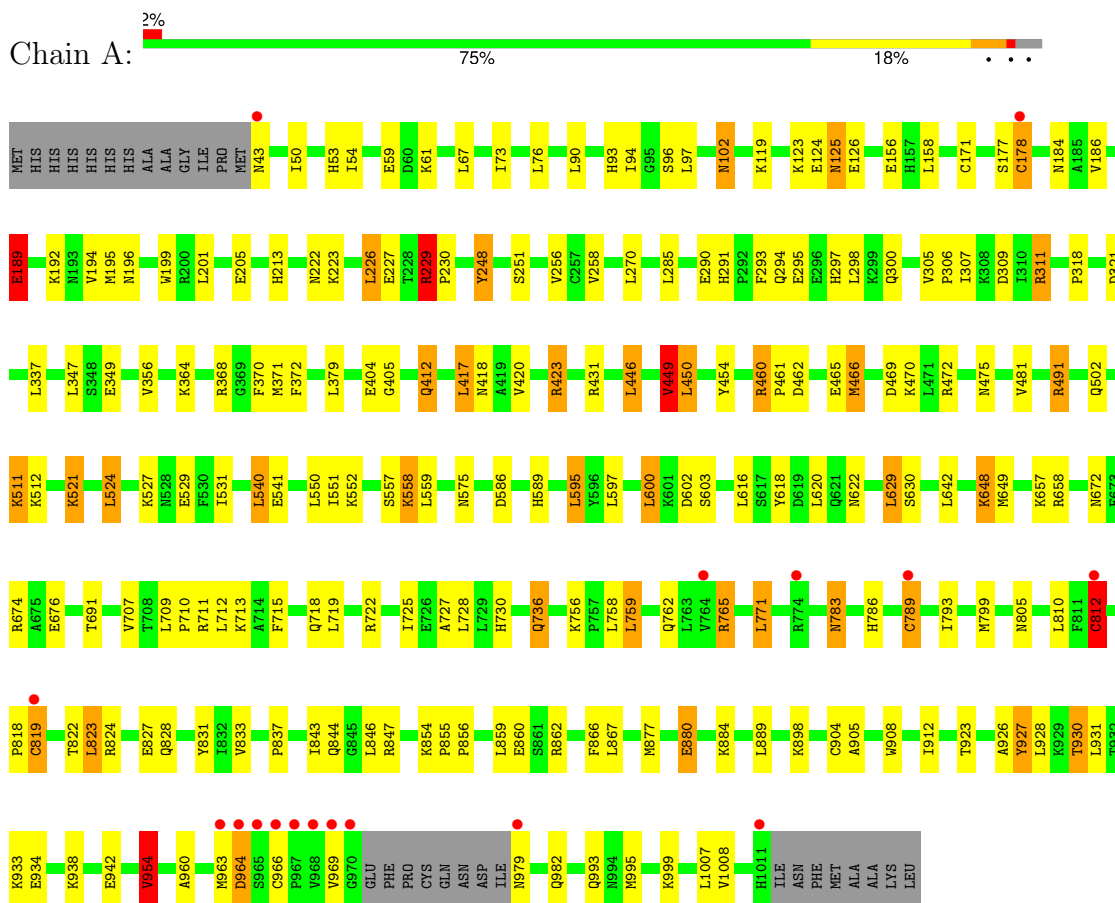
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total	O	0	0
			285	285		
4	B	283	Total	O	0	0
			283	283		

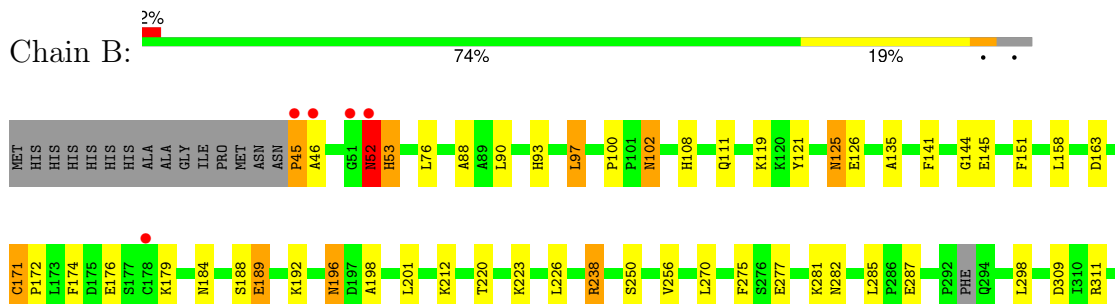
3 Residue-property plots

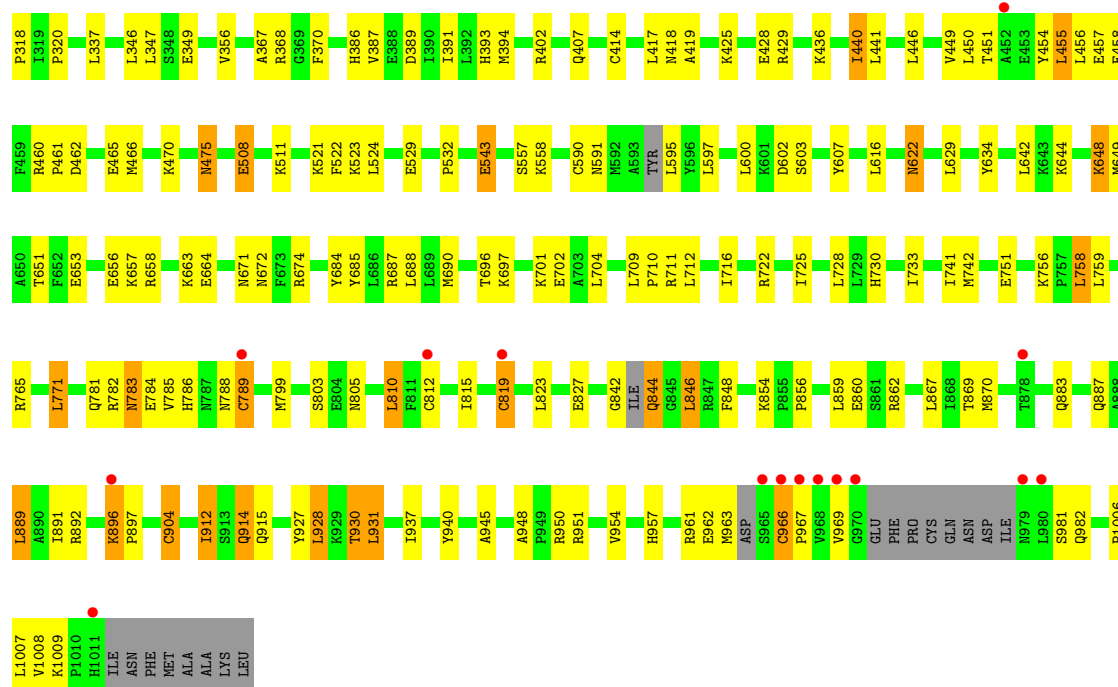
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

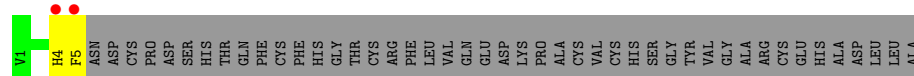


• Molecule 1: Insulin-degrading enzyme

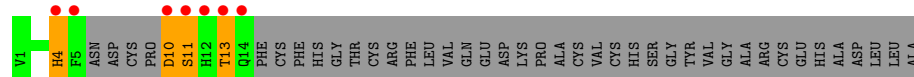




• Molecule 2: Protransforming growth factor alpha



• Molecule 2: Protransforming growth factor alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	262.17Å 262.17Å 90.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.30) 99.8 (50.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.231 0.196 , 0.234	Depositor DCC
R_{free} test set	7893 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16297	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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	1.29	15/8036 (0.2%)	1.20	25/10871 (0.2%)
1	B	1.26	14/7961 (0.2%)	1.20	32/10765 (0.3%)
2	C	1.36	0/35	1.41	0/47
2	D	1.70	2/82 (2.4%)	1.43	0/109
All	All	1.28	31/16114 (0.2%)	1.20	57/21792 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLU	CD-OE2	11.46	1.47	1.25
1	A	812	CYS	CB-SG	-8.62	1.52	1.81
1	A	258	VAL	CA-CB	7.87	1.64	1.54
1	A	819	CYS	CB-SG	-7.62	1.56	1.81
1	A	189	GLU	CB-CG	7.04	1.73	1.52
1	A	189	GLU	CA-CB	6.95	1.64	1.53
1	A	189	GLU	CD-OE2	6.57	1.37	1.25
1	A	905	ALA	CA-CB	6.57	1.63	1.53
1	B	590	CYS	CB-SG	-6.24	1.60	1.81
1	B	590	CYS	N-CA	-6.23	1.39	1.46
2	D	13	THR	CA-CB	6.16	1.63	1.53
1	B	716	ILE	CA-CB	6.16	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	741	ILE	CA-CB	6.06	1.61	1.54
1	A	926	ALA	CA-CB	6.05	1.62	1.53
1	A	178	CYS	CB-SG	-6.03	1.61	1.81
1	A	789	CYS	CB-SG	-6.01	1.61	1.81
1	B	789	CYS	CB-SG	-5.74	1.62	1.81
2	D	4	HIS	CA-C	5.66	1.60	1.52
1	A	305	VAL	CA-C	5.58	1.57	1.53
1	B	854	LYS	CA-C	5.37	1.59	1.53
1	B	475	ASN	CA-CB	5.35	1.60	1.53
1	B	189	GLU	CD-OE1	5.24	1.35	1.25
1	A	420	VAL	CA-CB	5.24	1.60	1.54
1	B	419	ALA	CA-CB	5.23	1.61	1.53
1	B	651	THR	CA-CB	5.21	1.61	1.53
1	B	220	THR	CA-CB	5.21	1.61	1.53
1	B	819	CYS	CB-SG	-5.17	1.64	1.81
1	B	690	MET	SD-CE	-5.17	1.66	1.79
1	A	927	TYR	CA-C	5.10	1.59	1.52
1	A	189	GLU	N-CA	5.04	1.52	1.46
1	A	833	VAL	CA-CB	5.00	1.60	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	GLU	CG-CD-OE1	-11.00	93.11	118.40
1	B	189	GLU	CG-CD-OE2	10.87	143.40	118.40
1	A	189	GLU	N-CA-CB	10.33	124.99	110.01
1	B	189	GLU	CB-CG-CD	9.08	128.04	112.60
1	A	189	GLU	CA-CB-CG	8.49	131.08	114.10
1	A	812	CYS	CB-CA-C	-7.72	98.76	110.88
1	B	456	LEU	N-CA-C	-7.64	96.47	109.24
1	A	954	VAL	CB-CA-C	-7.56	98.85	110.50
1	B	188	SER	CA-C-N	7.42	130.55	120.54
1	B	188	SER	C-N-CA	7.42	130.55	120.54
1	A	449	VAL	CB-CA-C	-7.22	100.97	112.16
1	A	854	LYS	CA-C-N	-7.07	114.57	119.66
1	A	854	LYS	C-N-CA	-7.07	114.57	119.66
1	B	429	ARG	CA-C-N	6.96	126.48	119.24
1	B	429	ARG	C-N-CA	6.96	126.48	119.24
1	B	904	CYS	CB-CA-C	-6.56	100.58	110.88
1	A	818	PRO	CA-C-N	-6.43	110.35	121.66
1	A	818	PRO	C-N-CA	-6.43	110.35	121.66
1	B	455	LEU	CB-CA-C	6.41	121.25	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	TYR	N-CA-C	6.31	117.82	111.07
1	B	171	CYS	N-CA-C	6.26	119.75	108.55
1	B	414	CYS	CB-CA-C	-6.24	101.09	110.88
1	A	311	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	B	966	CYS	CA-C-N	6.12	127.50	119.84
1	B	966	CYS	C-N-CA	6.12	127.50	119.84
1	A	460	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	B	751	GLU	N-CA-C	5.92	117.42	110.97
1	A	248	TYR	N-CA-C	5.87	120.57	113.41
1	A	405	GLY	CA-C-N	5.83	125.76	119.76
1	A	405	GLY	C-N-CA	5.83	125.76	119.76
1	A	942	GLU	N-CA-C	5.81	118.84	111.69
1	B	789	CYS	CA-CB-SG	-5.72	101.24	114.40
1	B	789	CYS	CB-CA-C	-5.68	99.88	109.83
1	B	915	GLN	N-CA-C	-5.67	106.71	113.97
1	A	189	GLU	CG-CD-OE1	-5.62	105.48	118.40
1	B	45	PRO	CA-C-N	5.54	131.36	122.83
1	B	45	PRO	C-N-CA	5.54	131.36	122.83
1	A	860	GLU	N-CA-C	5.54	117.31	111.28
1	B	844	GLN	N-CA-C	5.51	126.44	111.00
1	B	981	SER	N-CA-C	5.46	117.77	110.35
1	B	812	CYS	N-CA-C	5.43	117.62	111.11
1	A	884	LYS	N-CA-C	-5.41	105.47	111.36
1	A	812	CYS	CA-CB-SG	-5.40	101.97	114.40
1	A	96	SER	N-CA-C	5.38	122.26	110.80
1	B	275	PHE	N-CA-C	5.36	120.69	113.72
1	B	387	VAL	N-CA-C	5.35	116.07	110.62
1	B	590	CYS	CA-CB-SG	-5.34	102.12	114.40
1	A	311	ARG	CB-CA-C	-5.34	102.83	110.62
1	B	1009	LYS	CA-C-N	5.31	125.60	119.92
1	B	1009	LYS	C-N-CA	5.31	125.60	119.92
1	A	812	CYS	N-CA-C	5.23	116.67	111.07
1	A	229	ARG	CA-C-N	-5.20	113.57	119.28
1	A	229	ARG	C-N-CA	-5.20	113.57	119.28
1	B	904	CYS	N-CA-C	5.17	116.60	111.07
1	A	551	ILE	N-CA-C	-5.06	108.04	112.90
1	B	100	PRO	CA-C-N	5.06	124.72	119.56
1	B	100	PRO	C-N-CA	5.06	124.72	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	964	ASP	Peptide
1	B	52	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7840	0	7761	127	0
1	B	7771	0	7675	126	0
2	C	35	0	34	4	0
2	D	81	0	71	4	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	285	0	0	12	0
4	B	283	0	0	8	0
All	All	16297	0	15541	256	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 8.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:HIS:HB3	2:C:5:PHE:HA	1.27	1.09
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.13	1.07
1:A:819:CYS:HB3	1:A:866:PHE:CZ	1.93	1.02
1:B:46:ALA:HA	4:B:1254:HOH:O	1.58	1.02
2:C:4:HIS:HB3	2:C:5:PHE:CA	1.97	0.95
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.12	0.95
1:A:819:CYS:HB3	1:A:866:PHE:CE2	2.06	0.91
1:B:93:HIS:CE1	1:B:368:ARG:HH21	1.92	0.88
1:B:102:ASN:HD22	1:B:102:ASN:H	1.22	0.88
1:B:425:LYS:HE2	1:B:428:GLU:OE2	1.74	0.87
1:A:934:GLU:HG3	1:B:53:HIS:NE2	1.90	0.86
1:A:294:GLN:H	1:A:297:HIS:HD2	1.24	0.85
1:A:730:HIS:HD2	1:A:904:CYS:SG	1.99	0.85
1:A:789:CYS:SG	1:A:856:PRO:HD3	2.17	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:HIS:HD2	1:B:904:CYS:SG	2.00	0.84
1:B:782:ARG:HD2	4:B:1227:HOH:O	1.78	0.83
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.22	0.83
1:B:174:PHE:O	1:B:238:ARG:HD2	1.80	0.81
1:A:102:ASN:H	1:A:102:ASN:HD22	1.30	0.80
1:A:491:ARG:HH11	1:A:491:ARG:CG	1.94	0.80
1:A:730:HIS:CD2	1:A:904:CYS:SG	2.74	0.79
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.64	0.78
1:B:309:ASP:H	1:B:672:ASN:HD21	1.30	0.77
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.67	0.76
1:A:880:GLU:HB3	1:B:457:GLU:HG2	1.68	0.76
1:B:730:HIS:CD2	1:B:904:CYS:SG	2.80	0.73
1:A:59:GLU:OE2	1:A:423:ARG:NH1	2.22	0.72
2:C:4:HIS:CB	2:C:5:PHE:HA	2.15	0.72
1:A:53:HIS:HE1	4:A:24:HOH:O	1.72	0.72
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.20	0.72
1:A:603:SER:OG	1:A:648:LYS:HE3	1.89	0.71
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.87	0.71
1:B:125:ASN:HD22	1:B:125:ASN:H	1.38	0.71
1:B:789:CYS:SG	1:B:856:PRO:HD3	2.31	0.70
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.90	0.70
1:B:927:TYR:O	1:B:930:THR:HB	1.92	0.70
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.90	0.69
1:A:491:ARG:HG3	1:A:491:ARG:NH1	1.94	0.69
1:A:125:ASN:H	1:A:125:ASN:HD22	1.37	0.69
1:A:184:ASN:HD21	1:A:223:LYS:NZ	1.91	0.69
1:B:461:PRO:O	1:B:465:GLU:HG3	1.93	0.68
1:A:309:ASP:H	1:A:672:ASN:HD21	1.39	0.68
1:A:475:ASN:HB3	4:A:1214:HOH:O	1.93	0.68
1:B:603:SER:OG	1:B:648:LYS:HE3	1.93	0.68
1:A:674:ARG:HD2	4:A:1173:HOH:O	1.94	0.68
1:B:896:LYS:HD3	1:B:897:PRO:HD2	1.77	0.67
1:A:184:ASN:HD21	1:A:223:LYS:HZ2	1.40	0.66
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.77	0.66
1:A:222:ASN:O	1:A:226:LEU:HB2	1.95	0.66
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.11	0.66
1:B:887:GLN:HE21	1:B:891:ILE:HD11	1.61	0.66
1:A:541:GLU:OE2	1:A:736:GLN:NE2	2.28	0.65
1:A:927:TYR:O	1:A:930:THR:HB	1.97	0.65
1:A:979:ASN:ND2	4:A:1203:HOH:O	2.28	0.65
1:B:815:ILE:O	1:B:819:CYS:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:NH1	4:A:1257:HOH:O	2.28	0.64
1:B:815:ILE:HG22	1:B:870:MET:HG2	1.79	0.64
1:A:771:LEU:HD21	1:A:954:VAL:HG22	1.79	0.63
1:B:771:LEU:HD21	1:B:954:VAL:CG2	2.27	0.63
1:A:229:ARG:CB	1:A:229:ARG:HH11	2.12	0.63
1:A:321:ASP:OD2	1:A:371:MET:HE3	1.99	0.63
1:B:309:ASP:H	1:B:672:ASN:ND2	1.96	0.62
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.31	0.62
1:B:386:HIS:HE1	4:B:1104:HOH:O	1.81	0.62
1:A:819:CYS:HB2	1:A:823:LEU:HD22	1.81	0.62
1:B:805:ASN:HD22	1:B:844:GLN:HE22	1.48	0.62
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.81	0.62
1:B:111:GLN:HE21	2:D:13:THR:HG23	1.64	0.62
1:A:309:ASP:H	1:A:672:ASN:ND2	1.98	0.61
1:A:827:GLU:OE1	1:A:862:ARG:HD3	1.99	0.61
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.82	0.61
1:A:511:LYS:NZ	4:A:1233:HOH:O	2.32	0.61
1:B:671:ASN:OD1	1:B:701:LYS:HE3	1.99	0.61
1:B:782:ARG:CD	4:B:1227:HOH:O	2.44	0.61
1:B:827:GLU:OE1	1:B:862:ARG:CD	2.49	0.61
1:B:591:ASN:O	1:B:595:LEU:HB2	2.01	0.61
1:B:102:ASN:H	1:B:102:ASN:ND2	1.98	0.60
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.83	0.60
1:A:196:ASN:HD22	1:A:199:TRP:H	1.49	0.59
1:B:174:PHE:O	1:B:238:ARG:CD	2.50	0.59
1:B:782:ARG:NH1	1:B:961:ARG:O	2.34	0.59
1:B:111:GLN:NE2	2:D:13:THR:HG23	2.16	0.59
1:A:349:GLU:OE2	1:A:521:LYS:HG2	2.03	0.58
1:B:121:TYR:OH	1:B:163:ASP:OD1	2.17	0.58
1:B:600:LEU:HD11	1:B:648:LYS:HB3	1.84	0.58
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.03	0.58
1:B:783:ASN:HD22	1:B:785:VAL:H	1.51	0.58
1:A:461:PRO:O	1:A:465:GLU:HG3	2.04	0.57
1:A:194:VAL:HG12	1:A:195:MET:HE2	1.88	0.56
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.88	0.56
1:B:783:ASN:ND2	1:B:785:VAL:H	2.04	0.56
1:B:783:ASN:ND2	1:B:786:HIS:H	2.02	0.56
1:B:602:ASP:OD1	1:B:658:ARG:HD3	2.05	0.56
1:B:722:ARG:HB3	1:B:758:LEU:HD13	1.87	0.56
1:A:491:ARG:CG	1:A:491:ARG:NH1	2.62	0.55
1:A:805:ASN:HD22	1:A:844:GLN:HE22	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.52	0.55
1:B:309:ASP:N	1:B:672:ASN:HD21	2.03	0.55
1:B:97:LEU:HB2	1:B:144:GLY:O	2.07	0.54
1:B:815:ILE:HG22	1:B:870:MET:CG	2.37	0.54
1:A:595:LEU:HD23	1:A:707:VAL:HG11	1.90	0.54
1:B:126:GLU:HG3	4:B:1270:HOH:O	2.06	0.54
1:A:229:ARG:HH11	1:A:229:ARG:HB3	1.72	0.53
1:A:527:LYS:HE2	4:A:1087:HOH:O	2.08	0.53
1:A:783:ASN:ND2	1:A:786:HIS:H	2.06	0.53
1:A:124:GLU:OE2	1:A:178:CYS:HB3	2.08	0.53
1:B:788:ASN:ND2	4:B:1156:HOH:O	2.40	0.53
1:A:827:GLU:OE1	1:A:862:ARG:CD	2.56	0.52
1:A:469:ASP:OD1	1:A:472:ARG:NH2	2.37	0.52
1:A:307:ILE:O	1:A:674:ARG:NH2	2.43	0.52
1:B:466:MET:HE2	1:B:470:LYS:HZ3	1.74	0.52
1:B:508:GLU:CD	1:B:508:GLU:H	2.17	0.52
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.92	0.52
1:A:736:GLN:H	1:A:736:GLN:CD	2.18	0.51
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.37	0.51
1:A:446:LEU:O	1:A:449:VAL:HG22	2.11	0.51
1:B:803:SER:HA	1:B:927:TYR:CE2	2.46	0.51
1:A:93:HIS:HE1	1:A:368:ARG:NH2	2.01	0.51
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.93	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.45	0.50
1:A:293:PHE:CE2	1:A:372:PHE:HE2	2.30	0.50
1:A:550:LEU:HD11	1:A:558:LYS:HG2	1.94	0.50
1:B:102:ASN:HD22	1:B:102:ASN:N	2.00	0.50
1:B:349:GLU:CD	1:B:521:LYS:HD3	2.36	0.50
1:A:934:GLU:HG2	1:A:938:LYS:HD2	1.93	0.50
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.94	0.49
1:A:417:LEU:HD11	1:A:531:ILE:HG12	1.94	0.49
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.47	0.49
1:B:799:MET:HE1	1:B:1006:PRO:HG2	1.94	0.49
1:A:205:GLU:OE2	1:A:364:LYS:NZ	2.44	0.49
1:B:93:HIS:HD2	1:B:145:GLU:O	1.95	0.49
1:B:622:ASN:HD22	1:B:622:ASN:H	1.60	0.49
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.13	0.48
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.47	0.48
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.61	0.48
1:A:466:MET:HE2	1:A:466:MET:C	2.37	0.48
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.95	0.48
1:A:466:MET:HE2	1:A:466:MET:O	2.13	0.48
1:A:186:VAL:HA	1:A:189:GLU:HG3	1.96	0.48
1:B:196:ASN:C	1:B:196:ASN:HD22	2.22	0.48
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.96	0.48
1:B:688:LEU:HD13	1:B:696:THR:HG22	1.94	0.48
1:A:822:THR:O	1:A:827:GLU:HG3	2.14	0.48
4:A:1056:HOH:O	1:B:53:HIS:HB3	2.13	0.48
1:B:52:ASN:HB3	1:B:53:HIS:HD2	1.79	0.48
1:B:196:ASN:ND2	1:B:198:ALA:H	2.12	0.48
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.97	0.48
1:B:349:GLU:OE2	1:B:521:LYS:HD3	2.13	0.47
1:A:54:ILE:HG22	1:A:450:LEU:HD22	1.95	0.47
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.96	0.47
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.95	0.47
1:A:602:ASP:OD1	1:A:658:ARG:HD3	2.14	0.47
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.96	0.47
1:A:812:CYS:SG	1:A:837:PRO:HD3	2.55	0.47
2:D:10:ASP:HA	2:D:11:SER:HA	1.51	0.47
1:A:603:SER:OG	1:A:648:LYS:CE	2.61	0.46
1:A:819:CYS:CB	1:A:866:PHE:CZ	2.83	0.46
1:A:73:ILE:HG13	1:A:251:SER:HB2	1.97	0.46
1:B:451:THR:HB	1:B:455:LEU:HD12	1.96	0.46
1:B:543:GLU:CD	1:B:543:GLU:H	2.24	0.46
1:A:622:ASN:HD22	1:A:622:ASN:H	1.64	0.46
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.51	0.46
1:B:674:ARG:HD3	4:B:25:HOH:O	2.16	0.46
1:A:298:LEU:HD21	1:A:318:PRO:HG3	1.98	0.46
1:A:960:ALA:HB3	1:A:963:MET:HG3	1.97	0.46
1:B:846:LEU:HD13	1:B:848:PHE:CE1	2.51	0.46
1:A:119:LYS:HB3	1:A:171:CYS:SG	2.56	0.46
1:A:715:PHE:O	1:A:718:GLN:HB3	2.16	0.46
1:B:389:ASP:O	1:B:393:HIS:CD2	2.69	0.46
1:A:862:ARG:HD2	4:A:1204:HOH:O	2.16	0.46
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.98	0.46
1:A:765:ARG:HA	1:A:765:ARG:HD2	1.79	0.45
1:B:108:HIS:CE1	1:B:189:GLU:OE2	2.66	0.45
1:B:789:CYS:SG	1:B:963:MET:HE1	2.57	0.45
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.98	0.45
1:B:460:ARG:NH1	1:B:462:ASP:OD1	2.50	0.45
1:B:948:ALA:HB3	1:B:951:ARG:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LYS:NZ	4:A:1243:HOH:O	2.45	0.45
1:B:815:ILE:CG2	1:B:870:MET:HG2	2.46	0.45
2:C:4:HIS:CB	2:C:5:PHE:CA	2.81	0.45
1:A:877:MET:O	1:A:933:LYS:NZ	2.49	0.45
1:B:171:CYS:HA	1:B:172:PRO:HD2	1.73	0.45
1:A:306:PRO:HB3	1:A:481:VAL:CG1	2.46	0.45
1:A:412:GLN:HE21	1:A:412:GLN:HB3	1.52	0.45
1:B:320:PRO:HG2	1:B:466:MET:HE1	1.98	0.45
1:A:995:MET:O	1:A:999:LYS:HG3	2.17	0.44
1:B:532:PRO:HG3	1:B:634:TYR:CD2	2.52	0.44
1:A:470:LYS:HD2	4:A:1266:HOH:O	2.18	0.44
1:A:676:GLU:OE2	1:A:676:GLU:HA	2.17	0.44
1:B:725:ILE:HG21	1:B:742:MET:HE1	1.98	0.44
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.74	0.44
1:B:663:LYS:HE3	1:B:704:LEU:O	2.18	0.44
1:A:294:GLN:H	1:A:297:HIS:CD2	2.16	0.44
1:A:722:ARG:HA	1:A:756:LYS:O	2.18	0.44
1:B:402:ARG:NH2	4:B:1220:HOH:O	2.51	0.44
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.99	0.44
1:A:799:MET:CE	1:A:1008:VAL:HG22	2.46	0.44
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.52	0.44
1:A:466:MET:HE3	1:A:470:LYS:NZ	2.33	0.43
1:A:908:TRP:O	1:A:912:ILE:HG12	2.18	0.43
1:A:557:SER:HA	1:A:725:ILE:O	2.17	0.43
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.52	0.43
1:B:961:ARG:HD2	1:B:962:GLU:OE1	2.18	0.43
1:A:855:PRO:HB3	1:A:963:MET:CE	2.48	0.43
1:A:349:GLU:CD	1:A:521:LYS:HG2	2.44	0.43
1:B:912:ILE:HD12	1:B:912:ILE:HA	1.70	0.43
1:A:898:LYS:HE3	4:A:1042:HOH:O	2.18	0.43
1:A:189:GLU:HG2	1:A:831:TYR:CE1	2.53	0.43
1:A:575:ASN:ND2	1:A:630:SER:OG	2.51	0.43
1:A:575:ASN:O	1:A:727:ALA:HA	2.19	0.43
1:B:799:MET:HB2	1:B:799:MET:HE2	1.79	0.43
1:B:846:LEU:HD13	1:B:848:PHE:HE1	1.83	0.43
1:A:125:ASN:HD22	1:A:125:ASN:N	2.07	0.43
1:A:799:MET:HE2	1:A:799:MET:HB3	1.70	0.43
1:B:125:ASN:HD22	1:B:125:ASN:N	2.06	0.43
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.52	0.43
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.43
1:B:782:ARG:NH2	1:B:784:GLU:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:CYS:O	1:A:823:LEU:HB2	2.18	0.43
1:A:300:GLN:NE2	1:A:502:GLN:OE1	2.51	0.43
1:B:135:ALA:HA	1:B:892:ARG:NH2	2.34	0.42
1:B:466:MET:CE	1:B:470:LYS:HZ3	2.33	0.42
1:B:765:ARG:HA	1:B:765:ARG:HD2	1.80	0.42
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.54	0.42
1:A:586:ASP:OD1	1:A:589:HIS:CD2	2.72	0.42
1:A:213:HIS:NE2	1:A:290:GLU:O	2.50	0.42
1:A:418:ASN:HB3	1:A:454:TYR:O	2.19	0.42
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.57	0.42
1:A:600:LEU:HD11	1:A:649:MET:CB	2.50	0.42
1:B:815:ILE:O	1:B:819:CYS:CB	2.66	0.42
1:B:250:SER:HB2	1:B:281:LYS:HB2	2.02	0.42
1:B:466:MET:CE	1:B:470:LYS:NZ	2.83	0.42
1:A:227:GLU:C	1:A:230:PRO:HD2	2.45	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.19	0.41
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.50	0.41
1:B:45:PRO:HB2	1:B:46:ALA:H	1.54	0.41
1:A:404:GLU:HG3	1:A:524:LEU:CD1	2.51	0.41
1:A:618:TYR:HA	1:A:630:SER:O	2.20	0.41
1:B:172:PRO:HG2	1:B:174:PHE:CE1	2.56	0.41
1:B:367:ALA:HB3	1:B:370:PHE:CE2	2.54	0.41
1:B:436:LYS:HE3	1:B:440:ILE:HD13	2.03	0.41
1:B:842:GLY:HA3	1:B:1008:VAL:HG23	2.02	0.41
1:B:966:CYS:HA	1:B:967:PRO:HD2	1.81	0.41
1:B:298:LEU:HD21	1:B:318:PRO:HG3	2.02	0.41
1:A:102:ASN:H	1:A:102:ASN:ND2	2.09	0.41
1:B:391:ILE:O	1:B:394:MET:HB2	2.20	0.41
1:B:418:ASN:ND2	1:B:454:TYR:O	2.53	0.41
1:B:141:PHE:HA	2:D:11:SER:O	2.21	0.41
1:B:196:ASN:C	1:B:196:ASN:ND2	2.77	0.41
1:B:765:ARG:NH1	1:B:914:GLN:OE1	2.54	0.41
1:B:765:ARG:HH11	1:B:765:ARG:HD3	1.73	0.41
1:B:950:ARG:HH11	1:B:950:ARG:HD2	1.76	0.40
1:B:93:HIS:CE1	1:B:368:ARG:NH2	2.73	0.40
1:B:151:PHE:CD1	1:B:151:PHE:C	3.00	0.40
1:A:824:ARG:O	1:A:828:GLN:HA	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	957/990 (97%)	933 (98%)	23 (2%)	1 (0%)	48	60
1	B	943/990 (95%)	910 (96%)	31 (3%)	2 (0%)	43	55
2	C	3/50 (6%)	2 (67%)	1 (33%)	0	100	100
2	D	6/50 (12%)	4 (67%)	1 (17%)	1 (17%)	0	0
All	All	1909/2080 (92%)	1849 (97%)	56 (3%)	4 (0%)	43	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	4	HIS
1	A	964	ASP
1	B	53	HIS
1	B	52	ASN

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	857/883 (97%)	782 (91%)	75 (9%)	9	12
1	B	847/883 (96%)	773 (91%)	74 (9%)	9	12
2	C	4/43 (9%)	4 (100%)	0	100	100
2	D	10/43 (23%)	8 (80%)	2 (20%)	1	1
All	All	1718/1852 (93%)	1567 (91%)	151 (9%)	9	12

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	50	ILE
1	A	61	LYS
1	A	67	LEU
1	A	76	LEU
1	A	97	LEU
1	A	102	ASN
1	A	125	ASN
1	A	156	GLU
1	A	158	LEU
1	A	177	SER
1	A	189	GLU
1	A	192	LYS
1	A	201	LEU
1	A	226	LEU
1	A	229	ARG
1	A	270	LEU
1	A	285	LEU
1	A	295	GLU
1	A	337	LEU
1	A	347	LEU
1	A	356	VAL
1	A	412	GLN
1	A	417	LEU
1	A	423	ARG
1	A	431	ARG
1	A	446	LEU
1	A	449	VAL
1	A	450	LEU
1	A	466	MET
1	A	491	ARG
1	A	511	LYS
1	A	512	LYS
1	A	521	LYS
1	A	524	LEU
1	A	529	GLU
1	A	540	LEU
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	616	LEU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	642	LEU
1	A	648	LYS
1	A	657	LYS
1	A	691	THR
1	A	711	ARG
1	A	712	LEU
1	A	719	LEU
1	A	728	LEU
1	A	736	GLN
1	A	758	LEU
1	A	759	LEU
1	A	765	ARG
1	A	771	LEU
1	A	783	ASN
1	A	810	LEU
1	A	812	CYS
1	A	823	LEU
1	A	846	LEU
1	A	859	LEU
1	A	867	LEU
1	A	880	GLU
1	A	889	LEU
1	A	923	THR
1	A	928	LEU
1	A	930	THR
1	A	931	LEU
1	A	954	VAL
1	A	966	CYS
1	A	969	VAL
1	A	982	GLN
1	A	993	GLN
1	A	1007	LEU
1	B	76	LEU
1	B	97	LEU
1	B	102	ASN
1	B	119	LYS
1	B	125	ASN
1	B	158	LEU
1	B	192	LYS
1	B	196	ASN
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	212	LYS
1	B	226	LEU
1	B	238	ARG
1	B	270	LEU
1	B	277	GLU
1	B	282	ASN
1	B	285	LEU
1	B	287	GLU
1	B	337	LEU
1	B	347	LEU
1	B	356	VAL
1	B	407	GLN
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	458	GLU
1	B	475	ASN
1	B	508	GLU
1	B	511	LYS
1	B	523	LYS
1	B	524	LEU
1	B	529	GLU
1	B	543	GLU
1	B	557	SER
1	B	558	LYS
1	B	597	LEU
1	B	616	LEU
1	B	622	ASN
1	B	629	LEU
1	B	642	LEU
1	B	644	LYS
1	B	648	LYS
1	B	649	MET
1	B	653	GLU
1	B	657	LYS
1	B	687	ARG
1	B	702	GLU
1	B	711	ARG
1	B	712	LEU
1	B	728	LEU
1	B	733	ILE

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Mol	Chain	Res	Type
1	B	756	LYS
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	869	THR
1	B	883	GLN
1	B	889	LEU
1	B	896	LYS
1	B	912	ILE
1	B	914	GLN
1	B	928	LEU
1	B	930	THR
1	B	931	LEU
1	B	937	ILE
1	B	969	VAL
1	B	982	GLN
1	B	1007	LEU
2	D	10	ASP
2	D	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	93	HIS
1	A	102	ASN
1	A	125	ASN
1	A	157	HIS
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	332	HIS
1	A	363	GLN

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	412	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	621	GLN
1	A	622	ASN
1	A	672	ASN
1	A	730	HIS
1	A	783	ASN
1	A	805	ASN
1	A	828	GLN
1	A	841	ASN
1	A	883	GLN
1	A	957	HIS
1	A	979	ASN
1	B	93	HIS
1	B	102	ASN
1	B	111	GLN
1	B	125	ASN
1	B	129	GLN
1	B	184	ASN
1	B	196	ASN
1	B	231	ASN
1	B	294	GLN
1	B	300	GLN
1	B	376	ASN
1	B	386	HIS
1	B	393	HIS
1	B	412	GLN
1	B	475	ASN
1	B	499	GLN
1	B	502	GLN
1	B	575	ASN
1	B	589	HIS
1	B	621	GLN
1	B	622	ASN
1	B	672	ASN
1	B	718	GLN
1	B	730	HIS
1	B	743	GLN
1	B	783	ASN

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Mol	Chain	Res	Type
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	887	GLN
1	B	957	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	961/990 (97%)	-0.31	17 (1%) 67 69	14, 29, 45, 89	1 (0%)
1	B	955/990 (96%)	-0.19	20 (2%) 63 65	21, 33, 48, 94	0
2	C	5/50 (10%)	1.90	2 (40%) 1 0	32, 37, 65, 66	0
2	D	10/50 (20%)	3.23	7 (70%) 0 0	31, 61, 70, 73	0
All	All	1931/2080 (92%)	-0.23	46 (2%) 59 62	14, 31, 47, 94	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	968	VAL	8.1
1	A	967	PRO	7.9
1	B	968	VAL	7.7
1	B	969	VAL	7.7
1	A	774	ARG	7.5
1	A	970	GLY	6.6
1	B	967	PRO	6.4
1	B	970	GLY	6.0
1	B	980	LEU	6.0
2	D	12	HIS	5.7
1	A	969	VAL	5.3
1	B	45	PRO	5.2
2	D	5	PHE	5.0
2	D	14	GLN	4.9
2	D	13	THR	4.9
1	A	964	ASP	4.9
1	A	764	VAL	4.8
1	A	965	SER	4.7
2	C	5	PHE	4.6
2	D	10	ASP	4.5
1	B	966	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	965	SER	4.3
1	A	966	CYS	4.3
2	D	11	SER	4.0
1	B	878	THR	4.0
1	B	979	ASN	3.9
2	C	4	HIS	3.8
1	B	819	CYS	3.6
1	B	812	CYS	3.4
1	A	1011	HIS	3.4
1	B	178	CYS	2.9
1	B	52	ASN	2.8
2	D	4	HIS	2.8
1	B	789	CYS	2.8
1	B	1011	HIS	2.7
1	A	178	CYS	2.7
1	A	43	ASN	2.4
1	B	46	ALA	2.4
1	B	51	GLY	2.4
1	A	963	MET	2.4
1	A	789	CYS	2.2
1	B	896	LYS	2.2
1	A	979	ASN	2.1
1	B	452	ALA	2.1
1	A	812	CYS	2.0
1	A	819	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	1	1/1	0.95	0.36	2,2,2,2	0
3	ZN	D	51	1/1	0.99	0.34	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.