Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:18 AM GMT

PDB ID	:	3E50
Title	:	Crystal structure of human insulin degrading enzyme in complex with transforming growth factor-alpha
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

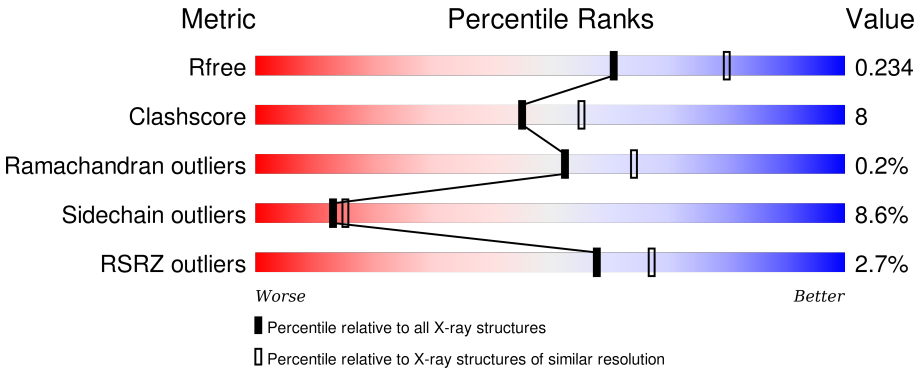
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	2% 75% 17%
1	B	990	2% 76% 16%
2	C	50	4% 6% 90%
2	D	50	14% 12% 80%

2 Entry composition (i)

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	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	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 35 22 7 6	0	0	0
2	D	10	Total C N O 81 50 15 16	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

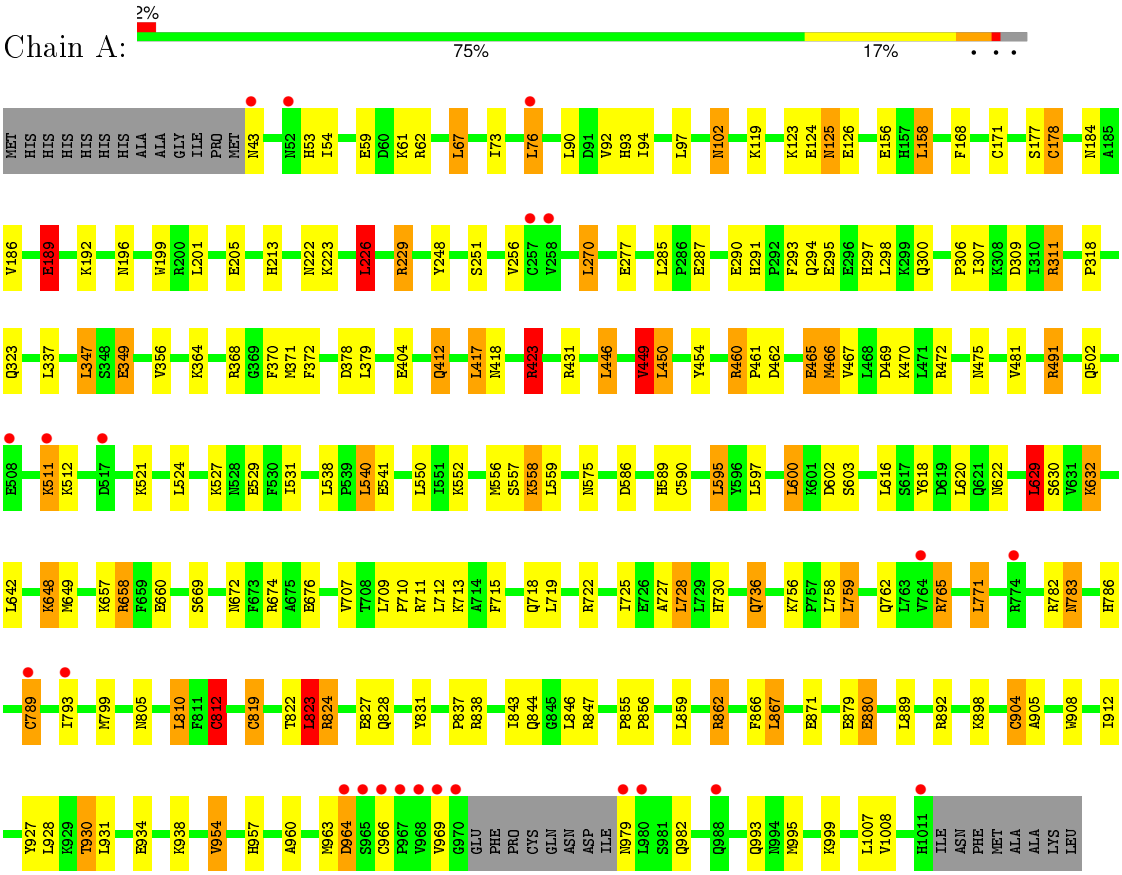
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	285	Total O 285 285	0	0
4	B	283	Total O 283 283	0	0

3 Residue-property plots (i)

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

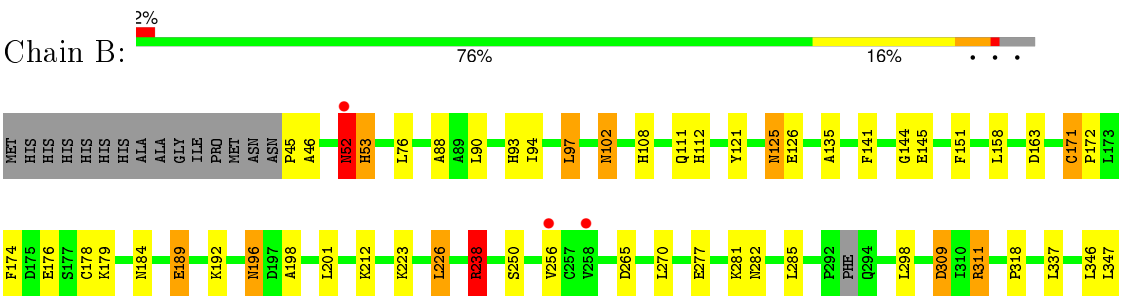
- Molecule 1: Insulin-degrading enzyme

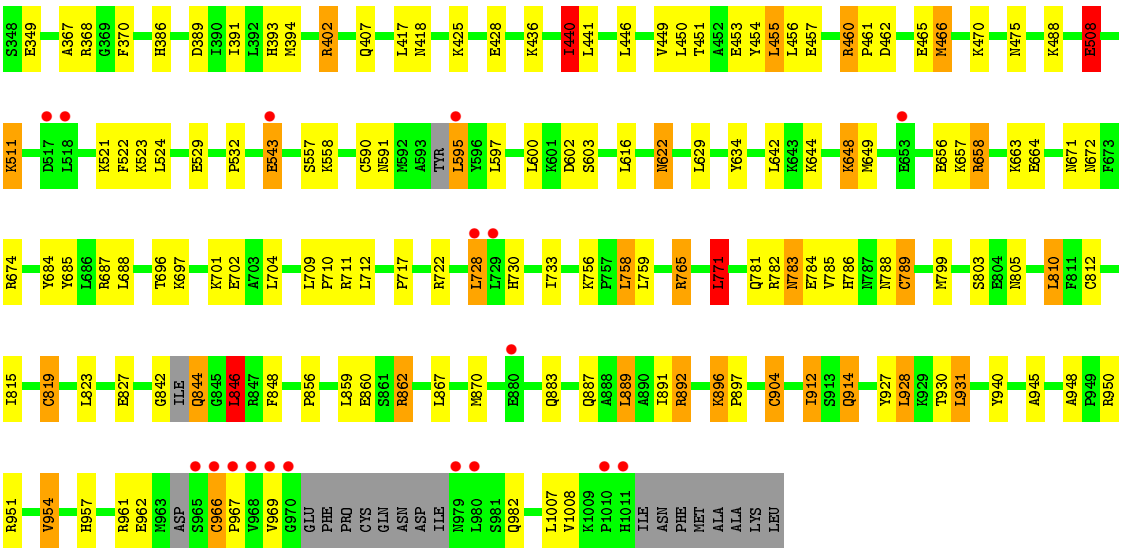
Chain A:



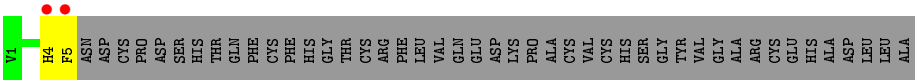
- Molecule 1: Insulin-degrading enzyme

Chain B:

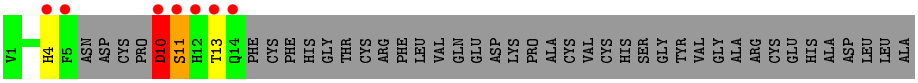




• Molecule 2: Protransforming growth factor alpha



• Molecule 2: Protransforming growth factor alpha



4 Data and refinement statistics (i)

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 22.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.30) 99.9 (22.19-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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 (5.29%)	DCC
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.5	EDS
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 157214 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.18	24/8036 (0.3%)	1.03	40/10871 (0.4%)
1	B	1.13	15/7961 (0.2%)	0.99	33/10765 (0.3%)
2	C	1.12	0/35	1.05	0/47
2	D	1.37	0/82	1.24	1/109 (0.9%)
All	All	1.16	39/16114 (0.2%)	1.01	74/21792 (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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	GLU	CD-OE2	19.52	1.47	1.25
1	A	812	CYS	CB-SG	-17.31	1.52	1.82
1	A	819	CYS	CB-SG	-15.39	1.56	1.82
1	B	590	CYS	CB-SG	-12.71	1.60	1.82
1	A	178	CYS	CB-SG	-12.30	1.61	1.82
1	A	789	CYS	CB-SG	-12.26	1.61	1.82
1	B	789	CYS	CB-SG	-11.72	1.62	1.82
1	A	189	GLU	CB-CG	11.28	1.73	1.52
1	A	189	GLU	CD-OE2	11.08	1.37	1.25
1	B	819	CYS	CB-SG	-10.63	1.64	1.82
1	A	904	CYS	CB-SG	-10.12	1.65	1.82
1	B	904	CYS	CB-SG	-10.11	1.65	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	CYS	CB-SG	-9.11	1.66	1.82
1	B	189	GLU	CD-OE1	8.78	1.35	1.25
1	B	189	GLU	CG-CD	8.21	1.64	1.51
1	B	812	CYS	CB-SG	-8.18	1.68	1.82
1	B	178	CYS	CB-SG	-7.96	1.68	1.82
1	B	508	GLU	CB-CG	7.42	1.66	1.52
1	B	508	GLU	CG-CD	7.38	1.63	1.51
1	B	453	GLU	CB-CG	6.60	1.64	1.52
1	A	879	GLU	CD-OE1	6.57	1.32	1.25
1	A	871	GLU	CG-CD	5.92	1.60	1.51
1	A	92	VAL	CB-CG1	5.85	1.65	1.52
1	B	511	LYS	CD-CE	5.76	1.65	1.51
1	A	669	SER	CB-OG	-5.75	1.34	1.42
1	A	879	GLU	CD-OE2	5.73	1.31	1.25
1	A	954	VAL	CB-CG2	-5.72	1.40	1.52
1	A	632	LYS	CD-CE	5.66	1.65	1.51
1	A	189	GLU	CG-CD	5.58	1.60	1.51
1	A	349	GLU	CG-CD	5.54	1.60	1.51
1	A	590	CYS	CB-SG	-5.46	1.73	1.81
1	A	287	GLU	CB-CG	5.38	1.62	1.52
1	A	905	ALA	CA-CB	5.37	1.63	1.52
1	A	277	GLU	CG-CD	5.33	1.59	1.51
1	A	168	PHE	CE2-CZ	5.31	1.47	1.37
1	A	660	GLU	CG-CD	5.19	1.59	1.51
1	A	871	GLU	CD-OE1	5.10	1.31	1.25
1	A	465	GLU	CD-OE2	5.06	1.31	1.25
1	B	954	VAL	CB-CG2	-5.03	1.42	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	A	460	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	B	189	GLU	CG-CD-OE1	-12.60	93.11	118.30
1	B	189	GLU	CG-CD-OE2	12.55	143.40	118.30
1	B	862	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	838	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	311	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	311	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	460	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	B	238	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	658	ARG	NE-CZ-NH2	-8.25	116.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	GLU	CA-CB-CG	8.04	131.08	113.40
1	A	189	GLU	N-CA-CB	8.00	124.99	110.60
1	A	824	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	862	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	658	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	238	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	789	CYS	CA-CB-SG	-7.09	101.24	114.00
1	B	460	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	862	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	823	LEU	CB-CG-CD1	6.89	122.72	111.00
1	B	402	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	423	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	812	CYS	CA-CB-SG	-6.68	101.97	114.00
1	A	954	VAL	CB-CA-C	-6.60	98.85	111.40
1	B	590	CYS	CA-CB-SG	-6.60	102.12	114.00
1	A	728	LEU	CA-CB-CG	6.48	130.19	115.30
1	A	189	GLU	CG-CD-OE1	-6.41	105.48	118.30
1	A	629	LEU	CB-CG-CD2	6.28	121.68	111.00
1	A	892	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	347	LEU	CB-CG-CD2	6.14	121.43	111.00
1	B	311	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	658	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	76	LEU	CB-CG-CD2	6.06	121.30	111.00
1	B	862	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	62	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	178	CYS	CA-CB-SG	-5.91	103.37	114.00
1	A	819	CYS	CA-CB-SG	-5.83	103.50	114.00
1	A	892	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	812	CYS	CB-CA-C	-5.82	98.76	110.40
1	B	455	LEU	CB-CA-C	5.82	121.25	110.20
1	A	189	GLU	CG-CD-OE2	5.80	129.89	118.30
2	D	10	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	B	844	GLN	N-CA-C	5.72	126.44	111.00
1	B	892	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	782	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	171	CYS	CA-CB-SG	-5.65	103.83	114.00
1	B	309	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	728	LEU	CB-CG-CD2	5.59	120.51	111.00
1	B	226	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	270	LEU	CB-CG-CD2	5.58	120.49	111.00
1	B	728	LEU	CB-CG-CD2	5.56	120.45	111.00
1	A	67	LEU	CB-CG-CD2	-5.52	101.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	838	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	449	VAL	CB-CA-C	-5.49	100.97	111.40
1	B	265	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	846	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	226	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	810	LEU	CB-CG-CD2	5.40	120.18	111.00
1	B	456	LEU	N-CA-C	-5.38	96.47	111.00
1	A	378	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	789	CYS	CA-CB-SG	-5.32	104.42	114.00
1	B	94	ILE	CG1-CB-CG2	-5.31	99.72	111.40
1	B	511	LYS	CD-CE-NZ	5.27	123.81	111.70
1	B	789	CYS	CB-CA-C	-5.26	99.88	110.40
1	A	158	LEU	CB-CG-CD2	5.24	119.91	111.00
1	B	226	LEU	CB-CG-CD1	5.23	119.89	111.00
1	B	771	LEU	CB-CG-CD1	5.22	119.87	111.00
1	B	819	CYS	CA-CB-SG	-5.15	104.73	114.00
1	B	595	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	867	LEU	CB-CG-CD1	5.13	119.72	111.00
1	B	189	GLU	CB-CG-CD	5.13	128.04	114.20
1	B	728	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	440	ILE	CG1-CB-CG2	-5.06	100.27	111.40

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 (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	7840	0	7761	122	0
1	B	7771	0	7675	120	0
2	C	35	0	34	4	0
2	D	81	0	71	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	245	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 (245) 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:H	1:B:102:ASN:HD22	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
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:HD22	1:A:102:ASN:H	1.30	0.80
1:A:491:ARG:CG	1:A:491:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:LEU:HD21	1:A:954:VAL:CG2	2.20	0.72
1:B:93:HIS:HE1	1:B:368:ARG:NH2	1.87	0.71
1:B:125:ASN:H	1:B:125:ASN:HD22	1.38	0.71
1:A:603:SER:OG	1:A:648:LYS:HE3	1.89	0.71
1:B:789:CYS:SG	1:B:856:PRO:HD3	2.31	0.70
1:B:927:TYR:O	1:B:930:THR:HB	1.92	0.70
1:B:827:GLU:OE1	1:B:862:ARG:HD3	1.90	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:HD22	1:A:125:ASN:H	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: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:112:HIS:NE2	1:B:189:GLU:OE2	2.29	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
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:HH11	1:A:229:ARG:CB	2.12	0.63
1:B:309:ASP:H	1:B:672:ASN:ND2	1.96	0.62
1:B:386:HIS:HE1	4:B:1104:HOH:O	1.81	0.62
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.31	0.62
1:A:799:MET:HE3	1:A:1008:VAL:HG22	1.82	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:B:111:GLN:HE21	2:D:13:THR:HG23	1.64	0.62
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:323:GLN:H	1:A:371:MET:HE3	1.67	0.58
1:A:461:PRO:O	1:A:465:GLU:HG3	2.04	0.57
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:B:121:TYR:OH	1:B:163:ASP:OD1	2.17	0.55
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
1:B:309:ASP:N	1:B:672:ASN:HD21	2.03	0.55
1:B:815:ILE:HG22	1:B:870:MET:CG	2.37	0.54
1:B:97:LEU:HB2	1:B:144:GLY:O	2.07	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:783:ASN:ND2	1:A:786:HIS:H	2.06	0.53
1:A:527:LYS:HE2	4:A:1087:HOH:O	2.08	0.53
1:A:184:ASN:HD21	1:A:223:LYS:HZ3	1.56	0.53
1:A:124:GLU:OE2	1:A:178:CYS:HB3	2.08	0.53
1:A:799:MET:HE1	1:A:1008:VAL:HA	1.90	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	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:OD1	1:A:589:HIS:HD2	1.92	0.52
1:B:176:GLU:OE1	1:B:179:LYS:NZ	2.37	0.51
1:B:803:SER:HA	1:B:927:TYR:CE2	2.46	0.51
1:A:446:LEU:O	1:A:449:VAL:HG22	2.11	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:184:ASN:HD21	1:A:223:LYS:HZ2	1.59	0.50
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.45	0.50
1:B:102:ASN:N	1:B:102:ASN:HD22	2.00	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:A:934:GLU:HG2	1:A:938:LYS:HD2	1.93	0.50
1:B:184:ASN:HD21	1:B:223:LYS:HZ1	1.58	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: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:H	1:B:622:ASN:HD22	1.60	0.49
1:B:602:ASP:OD1	1:B:658:ARG:CD	2.61	0.48
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.47	0.48
1:A:460:ARG:HD2	1:A:462:ASP:OD2	2.13	0.48
1:B:810:LEU:HG	1:B:928:LEU:HD21	1.94	0.48
1:B:860:GLU:OE2	1:B:957:HIS:HE1	1.95	0.48
1:A:186:VAL:HA	1:A:189:GLU:HG3	1.96	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
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:386:HIS:HD2	1:B:389:ASP:OD2	1.97	0.48
1:A:822:THR:O	1:A:827:GLU:HG3	2.14	0.48
1:B:196:ASN:ND2	1:B:198:ALA:H	2.12	0.48
1:B:508:GLU:CD	1:B:508:GLU:H	2.17	0.47
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:620:LEU:HD13	1:A:629:LEU:HG	1.95	0.47
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.96	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:736:GLN:H	1:A:736:GLN:CD	2.18	0.47
1:A:558:LYS:NZ	4:A:1243:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:819:CYS:CB	1:A:866:PHE:CZ	2.83	0.46
1:A:603:SER:OG	1:A:648:LYS:CE	2.61	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:A:466:MET:HE1	1:A:467:VAL:HA	1.98	0.46
1:A:622:ASN:H	1:A:622:ASN:HD22	1.64	0.46
1:B:674:ARG:HD3	4:B:25:HOH:O	2.16	0.46
1:B:346:LEU:HA	1:B:522:PHE:CE2	2.51	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:B:389:ASP:O	1:B:393:HIS:CD2	2.69	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:A:862:ARG:HD2	4:A:1204:HOH:O	2.16	0.46
1:B:466:MET:HE2	1:B:470:LYS:NZ	2.30	0.46
1:B:889:LEU:HB3	1:B:928:LEU:HD11	1.98	0.46
1:B:108:HIS:CE1	1:B:189:GLU:OE2	2.66	0.45
1:B:349:GLU:CD	1:B:521:LYS:HD3	2.36	0.45
1:A:765:ARG:HD2	1:A:765:ARG:HA	1.79	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
1:B:90:LEU:HD12	1:B:256:VAL:HG22	1.98	0.45
2:C:4:HIS:CB	2:C:5:PHE:CA	2.81	0.45
1:B:815:ILE:CG2	1:B:870:MET:HG2	2.46	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:HB3	1:A:412:GLN:HE21	1.52	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: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:B:402:ARG:NH2	4:B:1220:HOH:O	2.51	0.44
1:A:722:ARG:HA	1:A:756:LYS:O	2.18	0.44
1:A:709:LEU:HG	1:A:713:LYS:HE3	1.99	0.44
1:B:927:TYR:CE2	1:B:931:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:MET:CE	1:A:1008:VAL:HG22	2.46	0.44
1:A:908:TRP:O	1:A:912:ILE:HG12	2.18	0.43
1:B:961:ARG:HD2	1:B:962:GLU:OE1	2.18	0.43
1:B:685:TYR:CZ	1:B:781:GLN:HG3	2.52	0.43
1:A:557:SER:HA	1:A:725:ILE:O	2.17	0.43
1:A:855:PRO:HB3	1:A:963:MET:CE	2.48	0.43
1:B:912:ILE:HA	1:B:912:ILE:HD12	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:B:846:LEU:HD13	1:B:848:PHE:HE1	1.83	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:125:ASN:N	1:B:125:ASN:HD22	2.06	0.43
1:A:125:ASN:HD22	1:A:125:ASN:N	2.07	0.43
1:B:782:ARG:NH2	1:B:784:GLU:HG2	2.33	0.43
1:A:709:LEU:HB3	1:A:710:PRO:CD	2.44	0.43
1:A:460:ARG:NH1	1:A:462:ASP:OD1	2.52	0.43
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:196:ASN:HD22	1:B:196:ASN:C	2.22	0.42
1:B:940:TYR:CE1	1:B:945:ALA:HB2	2.54	0.42
1:B:765:ARG:HA	1:B:765:ARG:HD2	1.80	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:466:MET:CE	1:B:470:LYS:NZ	2.83	0.42
1:B:250:SER:HB2	1:B:281:LYS:HB2	2.02	0.42
1:B:45:PRO:HB2	1:B:46:ALA:H	1.54	0.41
1:A:799:MET:HG2	1:A:843:ILE:CD1	2.50	0.41
1:A:793:ILE:O	1:A:847:ARG:HA	2.19	0.41
1:A:618:TYR:HA	1:A:630:SER:O	2.20	0.41
1:B:543:GLU:CD	1:B:543:GLU:H	2.24	0.41
1:A:404:GLU:HG3	1:A:524:LEU:CD1	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:LYS:HE3	1:B:440:ILE:HD13	2.03	0.41
1:B:298:LEU:HD21	1:B:318:PRO:HG3	2.02	0.41
1:A:102:ASN:ND2	1:A:102:ASN:H	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: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:HD2	1:B:950:ARG:HH11	1.76	0.40
1:B:93:HIS:CE1	1:B:368:ARG:NH2	2.73	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 (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	957/990 (97%)	933 (98%)	23 (2%)	1 (0%)	56 68
1	B	943/990 (95%)	910 (96%)	31 (3%)	2 (0%)	52 64
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%)	52 64

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 (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	857/883 (97%)	784 (92%)	73 (8%)	13 16
1	B	847/883 (96%)	775 (92%)	72 (8%)	13 16
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%)	1571 (91%)	147 (9%)	13 15

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
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

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Mol	Chain	Res	Type
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	529	GLU
1	A	538	LEU
1	A	540	LEU
1	A	556	MET
1	A	558	LYS
1	A	595	LEU
1	A	597	LEU
1	A	600	LEU
1	A	616	LEU
1	A	629	LEU
1	A	632	LYS
1	A	642	LEU
1	A	648	LYS
1	A	657	LYS
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	928	LEU
1	A	930	THR

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Mol	Chain	Res	Type
1	A	931	LEU
1	A	957	HIS
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	125	ASN
1	B	158	LEU
1	B	192	LYS
1	B	196	ASN
1	B	201	LEU
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	337	LEU
1	B	347	LEU
1	B	407	GLN
1	B	417	LEU
1	B	440	ILE
1	B	446	LEU
1	B	450	LEU
1	B	466	MET
1	B	475	ASN
1	B	488	LYS
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

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Mol	Chain	Res	Type
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	657	LYS
1	B	687	ARG
1	B	702	GLU
1	B	711	ARG
1	B	712	LEU
1	B	717	PRO
1	B	728	LEU
1	B	733	ILE
1	B	756	LYS
1	B	758	LEU
1	B	759	LEU
1	B	765	ARG
1	B	771	LEU
1	B	783	ASN
1	B	799	MET
1	B	810	LEU
1	B	823	LEU
1	B	846	LEU
1	B	859	LEU
1	B	867	LEU
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	931	LEU
1	B	966	CYS
1	B	969	VAL
1	B	982	GLN
1	B	1007	LEU
2	D	10	ASP
2	D	11	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) 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	184	ASN
1	A	196	ASN
1	A	231	ASN
1	A	232	GLN
1	A	297	HIS
1	A	300	GLN
1	A	393	HIS
1	A	407	GLN
1	A	412	GLN
1	A	502	GLN
1	A	575	ASN
1	A	589	HIS
1	A	605	ASN
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	922	ASN
1	A	957	HIS
1	A	979	ASN
1	B	52	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	300	GLN
1	B	363	GLN
1	B	386	HIS
1	B	393	HIS
1	B	412	GLN
1	B	502	GLN

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Mol	Chain	Res	Type
1	B	575	ASN
1	B	589	HIS
1	B	605	ASN
1	B	621	GLN
1	B	622	ASN
1	B	672	ASN
1	B	730	HIS
1	B	783	ASN
1	B	788	ASN
1	B	805	ASN
1	B	828	GLN
1	B	841	ASN
1	B	887	GLN
1	B	922	ASN
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 carbohydrates 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, 95^{th} 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%)	-0.27	23 (2%)	62	71	17, 29, 45, 89	1 (0%)
1	B	955/990 (96%)	-0.25	21 (2%)	65	73	21, 33, 48, 95	0
2	C	5/50 (10%)	3.05	2 (40%)	0	0	32, 37, 65, 66	0
2	D	10/50 (20%)	2.71	7 (70%)	0	0	31, 61, 70, 73	0
All	All	1931/2080 (92%)	-0.24	53 (2%)	58	67	17, 31, 47, 95	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	5	PHE	9.9
1	A	967	PRO	7.3
1	A	964	ASP	6.5
2	D	4	HIS	6.3
2	D	5	PHE	6.0
1	A	965	SER	5.6
2	C	4	HIS	5.5
1	A	968	VAL	5.2
1	A	966	CYS	4.6
1	B	968	VAL	4.6
1	B	966	CYS	4.3
1	B	969	VAL	4.1
1	B	980	LEU	4.0
1	A	979	ASN	3.6
1	A	969	VAL	3.4
1	B	967	PRO	3.3
2	D	12	HIS	3.3
1	B	979	ASN	3.2
1	B	517	ASP	3.1
1	A	970	GLY	2.9
2	D	14	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	76	LEU	2.9
1	B	729	LEU	2.8
2	D	11	SER	2.7
1	B	970	GLY	2.7
1	A	517	ASP	2.7
1	A	793	ILE	2.5
1	B	965	SER	2.5
1	B	653	GLU	2.5
1	A	43	ASN	2.4
1	A	980	LEU	2.4
1	A	988	GLN	2.4
1	A	764	VAL	2.4
1	A	508	GLU	2.4
1	A	257	CYS	2.4
1	A	1011	HIS	2.4
1	A	511	LYS	2.4
2	D	10	ASP	2.3
1	B	1010	PRO	2.3
1	B	595	LEU	2.3
1	B	1011	HIS	2.3
1	B	543	GLU	2.3
2	D	13	THR	2.2
1	B	52	ASN	2.2
1	A	774	ARG	2.2
1	B	518	LEU	2.2
1	B	258	VAL	2.1
1	B	728	LEU	2.1
1	B	256	VAL	2.1
1	A	52	ASN	2.0
1	B	880	GLU	2.0
1	A	258	VAL	2.0
1	A	789	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	D	51	1/1	0.97	0.26	0.71	2,2,2,2	0
3	ZN	A	1	1/1	0.93	0.25	-	2,2,2,2	0

6.5 Other polymers

There are no such residues in this entry.