WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:31 PM GMT

PDB ID	:	3ZKW
Title	:	Periplasmic Binding Protein CeuE apo form
Authors	:	Raines, D.J.; Moroz, O.V.; Wilson, K.S.; Duhme-Klair, A.K.
Deposited on	:	2013-01-25
Resolution	:	1.71 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 (i)) 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 1.71 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		8
Ramachandran outliers		0.8%
Sidechain outliers		6.0%
RSRZ outliers		1.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
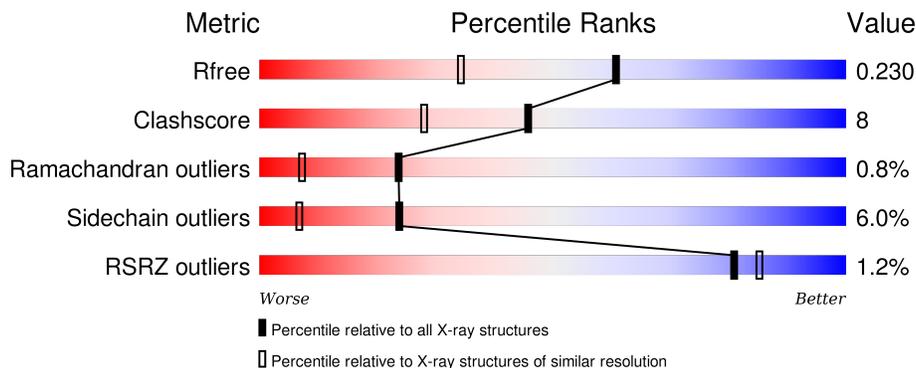
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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	287	% 84% 11% • •
1	C	287	2% 82% 13% • •
2	B	287	% 81% 16% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6763 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 ENTEROCHELIN UPTAKE PERIPLASMIC BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total 2220	C 1428	N 363	O 427	S 2	48	0	0
1	C	286	Total 2215	C 1424	N 363	O 426	S 2	17	0	0

- Molecule 2 is a protein called ENTEROCHELIN UPTAKE PERIPLASMIC BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	287	Total 2220	C 1428	N 363	O 427	S 2	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ILE	LEU	CONFLICT	UNP Q0P8Q4
B	41	ILE	LEU	CONFLICT	UNP Q0P8Q4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	38	Total 38	O 38	0	0
3	C	29	Total 29	O 29	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: ENTEROCHELIN UPTAKE PERIPLASMIC BINDING PROTEIN
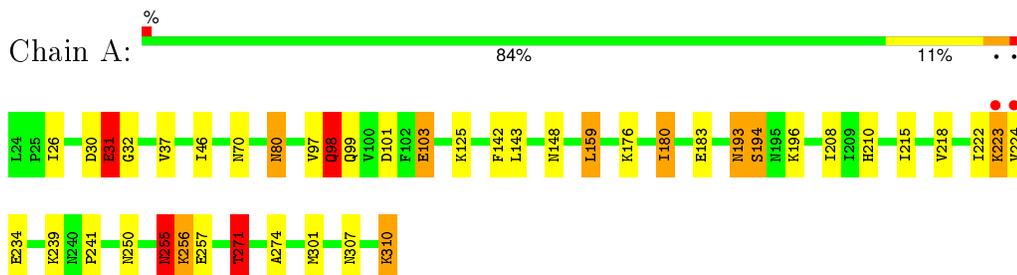
- Molecule 1: ENTEROCHELIN UPTAKE PERIPLASMIC BINDING PROTEIN
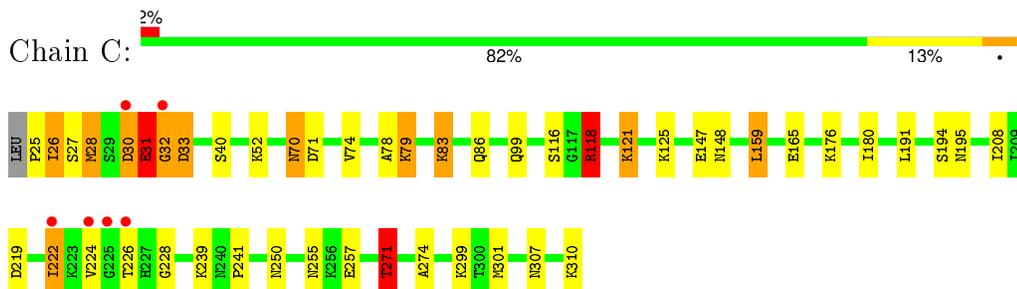
- Molecule 2: ENTEROCHELIN UPTAKE PERIPLASMIC BINDING PROTEIN
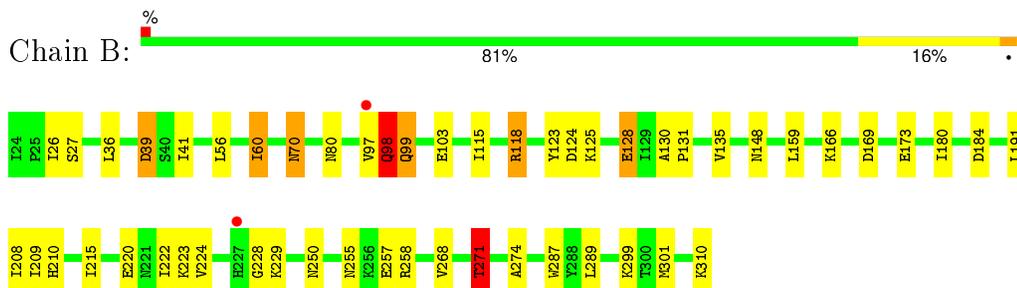
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.95Å 62.74Å 67.98Å 82.19° 76.74° 75.96°	Depositor
Resolution (Å)	65.93 – 1.71 65.93 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.93-1.71) 94.5 (65.93-1.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.227 0.198 , 0.230	Depositor DCC
R_{free} test set	4647 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 92847 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6763	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	1.61	10/2253 (0.4%)	1.27	24/3044 (0.8%)
1	C	1.34	9/2248 (0.4%)	1.08	15/3035 (0.5%)
2	B	1.20	7/2253 (0.3%)	1.34	14/3044 (0.5%)
All	All	1.39	26/6754 (0.4%)	1.23	53/9123 (0.6%)

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	2
1	C	0	1
2	B	1	2
All	All	1	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLU	CG-CD	-32.93	1.02	1.51
1	A	97	VAL	CA-C	30.88	2.33	1.52
1	C	147	GLU	CD-OE1	-30.66	0.92	1.25
1	C	147	GLU	CD-OE2	28.27	1.56	1.25
2	B	118	ARG	NE-CZ	24.22	1.64	1.33
1	A	234	GLU	CG-CD	-23.90	1.16	1.51
1	A	80	ASN	CA-CB	18.77	2.02	1.53
1	A	97	VAL	C-O	-18.53	0.88	1.23
2	B	99	GLN	CA-CB	-17.46	1.15	1.53
2	B	184	ASP	CA-CB	-16.11	1.18	1.53
1	A	256	LYS	C-N	-12.19	1.06	1.34
1	A	227	HIS	CB-CG	-11.81	1.28	1.50
1	A	97	VAL	CA-CB	10.99	1.77	1.54
1	C	31	GLU	N-CA	10.21	1.66	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	GLU	CG-CD	7.65	1.63	1.51
2	B	98	GLN	CA-CB	7.64	1.70	1.53
1	A	97	VAL	C-N	7.43	1.51	1.34
1	C	226	THR	CA-CB	-6.68	1.35	1.53
2	B	39	ASP	CB-CG	6.50	1.65	1.51
1	C	165	GLU	CD-OE2	6.27	1.32	1.25
1	C	299	LYS	CG-CD	5.89	1.72	1.52
1	C	83	LYS	CG-CD	5.80	1.72	1.52
2	B	287	TRP	CD2-CE2	5.50	1.48	1.41
1	A	255	ASN	C-N	-5.37	1.21	1.34
2	B	196	LYS	CD-CE	5.19	1.64	1.51
1	C	116	SER	CB-OG	5.08	1.48	1.42

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	118	ARG	NE-CZ-NH1	-29.46	105.57	120.30
2	B	118	ARG	CD-NE-CZ	-22.52	92.07	123.60
2	B	118	ARG	NE-CZ-NH2	19.95	130.27	120.30
1	A	97	VAL	CB-CA-C	-19.75	73.87	111.40
1	A	103	GLU	CB-CG-CD	14.22	152.59	114.20
1	A	255	ASN	O-C-N	-13.07	101.78	122.70
1	A	301	MET	CG-SD-CE	-13.04	79.33	100.20
2	B	99	GLN	CB-CA-C	11.92	134.24	110.40
2	B	98	GLN	CA-CB-CG	11.76	139.28	113.40
1	A	97	VAL	N-CA-C	-11.35	80.36	111.00
1	A	80	ASN	N-CA-CB	-10.60	91.52	110.60
1	A	97	VAL	CA-CB-CG2	-10.30	95.45	110.90
2	B	301	MET	CG-SD-CE	-10.25	83.81	100.20
1	A	226	THR	N-CA-CB	9.53	128.40	110.30
1	C	147	GLU	CG-CD-OE2	-8.77	100.76	118.30
1	A	143	LEU	CB-CG-CD1	-8.69	96.22	111.00
1	C	83	LYS	CG-CD-CE	8.62	137.77	111.90
1	A	196	LYS	CB-CG-CD	-7.83	91.25	111.60
2	B	99	GLN	CA-CB-CG	-7.71	96.44	113.40
1	A	98	GLN	N-CA-CB	7.57	124.22	110.60
1	C	159	LEU	CB-CG-CD1	7.44	123.64	111.00
2	B	39	ASP	CB-CG-OD1	7.07	124.66	118.30
2	B	271	THR	OG1-CB-CG2	7.03	126.17	110.00
1	C	226	THR	N-CA-CB	-7.03	96.95	110.30
1	A	255	ASN	CA-C-N	6.97	132.54	117.20
1	A	97	VAL	CA-CB-CG1	-6.90	100.56	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASN	N-CA-C	6.87	129.56	111.00
1	C	147	GLU	CG-CD-OE1	6.80	131.91	118.30
2	B	60	ILE	CG1-CB-CG2	-6.37	97.39	111.40
2	B	98	GLN	CB-CA-C	6.22	122.85	110.40
1	C	30	ASP	N-CA-C	6.20	127.73	111.00
1	C	28	MET	CG-SD-CE	6.14	110.03	100.20
1	A	101	ASP	CB-CG-OD1	6.06	123.75	118.30
2	B	258	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	97	VAL	C-N-CA	-5.98	106.76	121.70
1	A	234	GLU	CB-CG-CD	5.97	130.31	114.20
1	C	165	GLU	CA-CB-CG	5.81	126.18	113.40
2	B	271	THR	N-CA-CB	-5.71	99.46	110.30
1	A	226	THR	CA-CB-CG2	5.68	120.36	112.40
1	A	159	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	271	THR	N-CA-CB	-5.57	99.72	110.30
1	C	118	ARG	CG-CD-NE	5.55	123.45	111.80
1	C	271	THR	N-CA-CB	-5.45	99.95	110.30
1	A	31	GLU	N-CA-C	5.43	125.67	111.00
1	A	183	GLU	CG-CD-OE1	-5.37	107.56	118.30
1	C	31	GLU	N-CA-C	5.28	125.26	111.00
2	B	184	ASP	CB-CA-C	5.27	120.94	110.40
1	A	183	GLU	CG-CD-OE2	5.25	128.81	118.30
1	C	31	GLU	CA-C-N	5.25	126.71	116.20
1	C	176	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	C	165	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	A	176	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	C	301	MET	CG-SD-CE	-5.14	91.97	100.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	98	GLN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASN	Mainchain
1	A	80	ASN	Peptide
2	B	118	ARG	Sidechain
2	B	223	LYS	Peptide
1	C	32	GLY	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	2220	0	2271	25	0
1	C	2215	0	2275	41	0
2	B	2220	0	2276	38	0
3	A	41	0	0	0	0
3	B	38	0	0	3	0
3	C	29	0	0	2	0
All	All	6763	0	6822	102	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 (102) 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:C:224:VAL:HG21	1:C:228:GLY:HA2	1.44	0.99
1:A:26:ILE:H	1:A:148:ASN:HD21	1.07	0.96
1:A:250:ASN:HD22	1:A:255:ASN:HD22	1.18	0.91
1:A:30:ASP:O	1:A:31:GLU:OE1	1.90	0.89
2:B:26:ILE:H	2:B:148:ASN:HD21	1.19	0.89
1:C:224:VAL:HG21	1:C:228:GLY:CA	2.03	0.88
1:C:78:ALA:O	1:C:79:LYS:CB	2.20	0.86
1:C:27:SER:H	1:C:148:ASN:HD21	1.26	0.84
1:C:27:SER:HB2	3:C:2001:HOH:O	1.82	0.77
1:C:250:ASN:HD22	1:C:255:ASN:HD22	1.33	0.76
1:A:142:PHE:CE2	1:A:208:ILE:HD11	2.20	0.76
1:C:218:VAL:HG11	1:C:241:PRO:HB3	1.69	0.75
1:A:250:ASN:ND2	1:A:255:ASN:HD22	1.85	0.74
1:A:224:VAL:HG13	1:A:225:GLY:O	1.89	0.72
1:A:193:ASN:O	1:A:194:SER:HB3	1.89	0.71
2:B:250:ASN:HD22	2:B:255:ASN:HD22	1.39	0.71
1:C:78:ALA:O	1:C:79:LYS:HB3	1.91	0.70
1:A:250:ASN:HD22	1:A:255:ASN:ND2	1.90	0.69
1:C:25:PRO:HB2	1:C:40:SER:HB3	1.74	0.69
2:B:27:SER:HB2	1:C:121:LYS:HG3	1.74	0.69
2:B:70:ASN:HD22	2:B:70:ASN:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:VAL:CG2	1:C:228:GLY:H	2.08	0.66
1:C:27:SER:CB	3:C:2001:HOH:O	2.44	0.63
2:B:97:VAL:HG11	2:B:289:LEU:HD22	1.82	0.62
1:C:224:VAL:HG21	1:C:228:GLY:N	2.14	0.62
1:C:83:LYS:HA	1:C:86:GLN:HG2	1.80	0.62
1:C:194:SER:H	1:C:250:ASN:HD21	1.49	0.60
1:A:70:ASN:HD22	1:A:70:ASN:H	1.49	0.60
1:A:222:ILE:O	1:A:223:LYS:O	2.19	0.60
2:B:26:ILE:N	2:B:148:ASN:HD21	1.94	0.59
2:B:26:ILE:H	2:B:148:ASN:ND2	1.94	0.58
2:B:80:ASN:OD1	2:B:97:VAL:HG22	2.03	0.58
1:A:26:ILE:N	1:A:148:ASN:HD21	1.91	0.58
1:C:250:ASN:ND2	1:C:255:ASN:HD22	2.00	0.58
1:A:37:VAL:HG21	1:A:46:ILE:HD12	1.85	0.57
2:B:41:ILE:HG22	2:B:41:ILE:O	2.05	0.56
2:B:166:LYS:O	2:B:169:ASP:OD1	2.24	0.56
2:B:41:ILE:HG21	2:B:123:TYR:CG	2.41	0.56
1:C:307:ASN:ND2	1:C:310:LYS:NZ	2.54	0.55
1:C:219:ASP:CG	1:C:222:ILE:HD13	2.26	0.55
1:C:70:ASN:H	1:C:70:ASN:HD22	1.54	0.55
2:B:173:GLU:HG3	2:B:299:LYS:HE2	1.88	0.55
2:B:194:SER:H	2:B:250:ASN:HD21	1.54	0.54
1:A:26:ILE:H	1:A:148:ASN:ND2	1.90	0.54
1:C:32:GLY:O	1:C:33:ASP:HB3	2.07	0.54
2:B:250:ASN:ND2	2:B:255:ASN:HD22	2.05	0.54
2:B:56:LEU:HD12	2:B:115:ILE:HG22	1.91	0.53
1:A:271:THR:CG2	1:A:274:ALA:H	2.21	0.53
2:B:41:ILE:HG22	2:B:123:TYR:CE2	2.44	0.53
1:C:78:ALA:O	1:C:79:LYS:HB2	2.07	0.52
1:C:194:SER:N	1:C:250:ASN:HD21	2.07	0.51
2:B:130:ALA:HB1	2:B:131:PRO:HD2	1.92	0.51
2:B:60:ILE:HG13	2:B:135:VAL:HG21	1.92	0.51
2:B:210:HIS:HD2	2:B:215:ILE:O	1.94	0.51
2:B:80:ASN:OD1	2:B:97:VAL:N	2.33	0.51
1:A:30:ASP:C	1:A:31:GLU:OE1	2.49	0.50
1:A:222:ILE:O	1:A:223:LYS:C	2.49	0.50
2:B:222:ILE:HD12	2:B:229:LYS:CD	2.42	0.49
1:C:219:ASP:OD2	1:C:222:ILE:HD11	2.12	0.49
2:B:70:ASN:ND2	2:B:70:ASN:H	2.09	0.48
1:C:210:HIS:HD2	1:C:215:ILE:O	1.96	0.48
1:C:26:ILE:HG22	1:C:148:ASN:CG	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ASP:OD2	1:C:222:ILE:CD1	2.62	0.48
1:A:193:ASN:O	1:A:194:SER:CB	2.60	0.47
1:C:118:ARG:CG	1:C:118:ARG:HH11	2.28	0.47
1:C:271:THR:CG2	1:C:274:ALA:H	2.27	0.47
1:C:52:LYS:HA	1:C:74:VAL:HG13	1.97	0.47
2:B:222:ILE:HD12	2:B:229:LYS:HD3	1.96	0.47
2:B:194:SER:N	2:B:250:ASN:HD21	2.12	0.47
1:C:219:ASP:CG	1:C:222:ILE:CD1	2.83	0.47
1:A:271:THR:HG23	1:A:274:ALA:H	1.81	0.46
1:C:26:ILE:HG22	1:C:148:ASN:ND2	2.31	0.46
2:B:268:VAL:O	2:B:271:THR:HB	2.15	0.45
1:C:27:SER:H	1:C:148:ASN:ND2	2.04	0.45
1:C:30:ASP:O	1:C:31:GLU:HB2	2.16	0.45
1:A:210:HIS:HD2	1:A:215:ILE:O	2.00	0.45
2:B:41:ILE:HG22	2:B:123:TYR:CD2	2.52	0.45
2:B:271:THR:CG2	2:B:274:ALA:H	2.30	0.45
1:A:218:VAL:HG11	1:A:241:PRO:HB3	1.99	0.45
2:B:228:GLY:N	3:B:2024:HOH:O	1.72	0.44
1:C:307:ASN:ND2	1:C:310:LYS:HZ3	2.16	0.44
1:A:239:LYS:HA	1:A:239:LYS:HD3	1.90	0.44
2:B:124:ASP:O	2:B:128:GLU:OE1	2.36	0.43
1:A:224:VAL:HG11	1:A:228:GLY:HA2	1.99	0.43
1:A:180:ILE:HD12	1:A:180:ILE:C	2.39	0.43
1:C:32:GLY:O	1:C:33:ASP:CB	2.65	0.43
1:C:307:ASN:ND2	1:C:310:LYS:HZ1	2.16	0.43
2:B:27:SER:CB	1:C:121:LYS:HG3	2.45	0.43
2:B:228:GLY:CA	3:B:2024:HOH:O	2.45	0.42
2:B:97:VAL:HG11	2:B:289:LEU:CD2	2.49	0.42
2:B:208:ILE:CG2	2:B:209:ILE:N	2.80	0.42
2:B:41:ILE:CG2	2:B:123:TYR:CD2	3.02	0.42
1:C:222:ILE:N	1:C:222:ILE:CD1	2.83	0.42
1:A:30:ASP:OD1	1:A:32:GLY:HA2	2.20	0.42
2:B:208:ILE:HD13	2:B:208:ILE:HG21	1.59	0.41
2:B:220:GLU:OE2	3:B:2023:HOH:O	2.22	0.41
2:B:41:ILE:HD13	2:B:41:ILE:HG21	1.85	0.41
2:B:41:ILE:CG2	2:B:41:ILE:O	2.70	0.40
1:C:239:LYS:HA	1:C:239:LYS:HD3	1.97	0.40
1:A:307:ASN:HA	1:A:310:LYS:HG2	2.03	0.40
1:C:219:ASP:HB3	1:C:222:ILE:HD13	2.03	0.40
1:C:222:ILE:N	1:C:222:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

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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	285/287 (99%)	274 (96%)	8 (3%)	3 (1%)	17	4
1	C	284/287 (99%)	272 (96%)	9 (3%)	3 (1%)	17	4
2	B	285/287 (99%)	276 (97%)	8 (3%)	1 (0%)	39	20
All	All	854/861 (99%)	822 (96%)	25 (3%)	7 (1%)	24	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	223	LYS
1	A	194	SER
2	B	98	GLN
1	C	33	ASP
1	C	79	LYS
1	C	31	GLU

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	244/250 (98%)	232 (95%)	12 (5%)	31	10
1	C	244/250 (98%)	227 (93%)	17 (7%)	19	4
2	B	244/250 (98%)	229 (94%)	15 (6%)	23	6
All	All	732/750 (98%)	688 (94%)	44 (6%)	24	7

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	98	GLN
1	A	99	GLN
1	A	103	GLU
1	A	125	LYS
1	A	159	LEU
1	A	180	ILE
1	A	226	THR
1	A	256	LYS
1	A	257	GLU
1	A	271	THR
1	A	310	LYS
2	B	36	LEU
2	B	39	ASP
2	B	70	ASN
2	B	98	GLN
2	B	99	GLN
2	B	103	GLU
2	B	125	LYS
2	B	128	GLU
2	B	159	LEU
2	B	180	ILE
2	B	191	LEU
2	B	224	VAL
2	B	257	GLU
2	B	271	THR
2	B	310	LYS
1	C	26	ILE
1	C	28	MET
1	C	31	GLU
1	C	70	ASN
1	C	71	ASP
1	C	99	GLN
1	C	118	ARG
1	C	121	LYS
1	C	125	LYS
1	C	159	LEU
1	C	180	ILE
1	C	191	LEU
1	C	195	ASN
1	C	208	ILE
1	C	222	ILE

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Mol	Chain	Res	Type
1	C	257	GLU
1	C	271	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	90	ASN
1	A	99	GLN
1	A	148	ASN
1	A	172	ASN
1	A	210	HIS
1	A	216	ASN
1	A	250	ASN
2	B	70	ASN
2	B	86	GLN
2	B	148	ASN
2	B	210	HIS
2	B	250	ASN
1	C	70	ASN
1	C	90	ASN
1	C	148	ASN
1	C	210	HIS
1	C	216	ASN
1	C	250	ASN
1	C	307	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	286/287 (99%)	-0.23	2 (0%)	89	91	15, 27, 48, 70	14 (4%)
1	C	286/287 (99%)	-0.18	6 (2%)	67	71	15, 29, 48, 60	9 (3%)
2	B	287/287 (100%)	-0.28	2 (0%)	89	91	17, 26, 44, 64	7 (2%)
All	All	859/861 (99%)	-0.23	10 (1%)	81	85	15, 27, 47, 70	30 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	VAL	5.2
1	C	226	THR	3.6
1	C	224	VAL	2.7
1	C	225	GLY	2.6
1	C	222	ILE	2.5
2	B	97	VAL	2.5
1	C	32	GLY	2.5
1	A	223	LYS	2.4
1	C	30	ASP	2.1
2	B	227	HIS	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.