Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:10 AM GMT

PDB ID	:	2FYI
Title	:	Crystal Structure of the Cofactor-Binding Domain of the Cbl Transcriptional Regulator
Authors	:	Stec, E.; Neumann, P.; Wilkinson, A.J.; Brzozowski, A.M.; Bujacz, G.D.
Deposited on	:	2006-02-08
Resolution	:	2.80 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 ⓘ symbol.

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

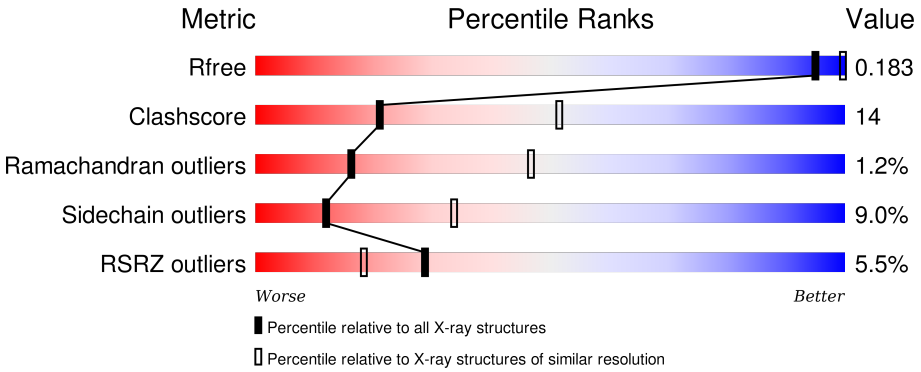
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	228	5% 65% 27% 5%
1	B	228	4% 69% 24% 5%
1	C	228	5% 66% 27% 7%
1	D	228	7% 68% 24% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7608 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 HTH-type transcriptional regulator cbl.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	4	0
			1807	1146	319	339	3			
1	B	223	Total	C	N	O	S	0	3	0
			1798	1139	318	338	3			
1	C	228	Total	C	N	O	S	0	3	0
			1834	1161	325	345	3			
1	D	223	Total	C	N	O	S	0	2	0
			1789	1132	315	339	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	LEU	-	CLONING ARTIFACT	UNP Q47083
A	81	VAL	-	CLONING ARTIFACT	UNP Q47083
A	82	PRO	-	CLONING ARTIFACT	UNP Q47083
A	83	ARG	-	CLONING ARTIFACT	UNP Q47083
A	84	GLY	-	CLONING ARTIFACT	UNP Q47083
A	85	SER	-	CLONING ARTIFACT	UNP Q47083
A	86	HIS	-	CLONING ARTIFACT	UNP Q47083
A	87	MET	-	CLONING ARTIFACT	UNP Q47083
B	80	LEU	-	CLONING ARTIFACT	UNP Q47083
B	81	VAL	-	CLONING ARTIFACT	UNP Q47083
B	82	PRO	-	CLONING ARTIFACT	UNP Q47083
B	83	ARG	-	CLONING ARTIFACT	UNP Q47083
B	84	GLY	-	CLONING ARTIFACT	UNP Q47083
B	85	SER	-	CLONING ARTIFACT	UNP Q47083
B	86	HIS	-	CLONING ARTIFACT	UNP Q47083
B	87	MET	-	CLONING ARTIFACT	UNP Q47083
C	80	LEU	-	CLONING ARTIFACT	UNP Q47083
C	81	VAL	-	CLONING ARTIFACT	UNP Q47083
C	82	PRO	-	CLONING ARTIFACT	UNP Q47083
C	83	ARG	-	CLONING ARTIFACT	UNP Q47083
C	84	GLY	-	CLONING ARTIFACT	UNP Q47083

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Chain	Residue	Modelled	Actual	Comment	Reference
C	85	SER	-	CLONING ARTIFACT	UNP Q47083
C	86	HIS	-	CLONING ARTIFACT	UNP Q47083
C	87	MET	-	CLONING ARTIFACT	UNP Q47083
D	80	LEU	-	CLONING ARTIFACT	UNP Q47083
D	81	VAL	-	CLONING ARTIFACT	UNP Q47083
D	82	PRO	-	CLONING ARTIFACT	UNP Q47083
D	83	ARG	-	CLONING ARTIFACT	UNP Q47083
D	84	GLY	-	CLONING ARTIFACT	UNP Q47083
D	85	SER	-	CLONING ARTIFACT	UNP Q47083
D	86	HIS	-	CLONING ARTIFACT	UNP Q47083
D	87	MET	-	CLONING ARTIFACT	UNP Q47083

- Molecule 2 is water.

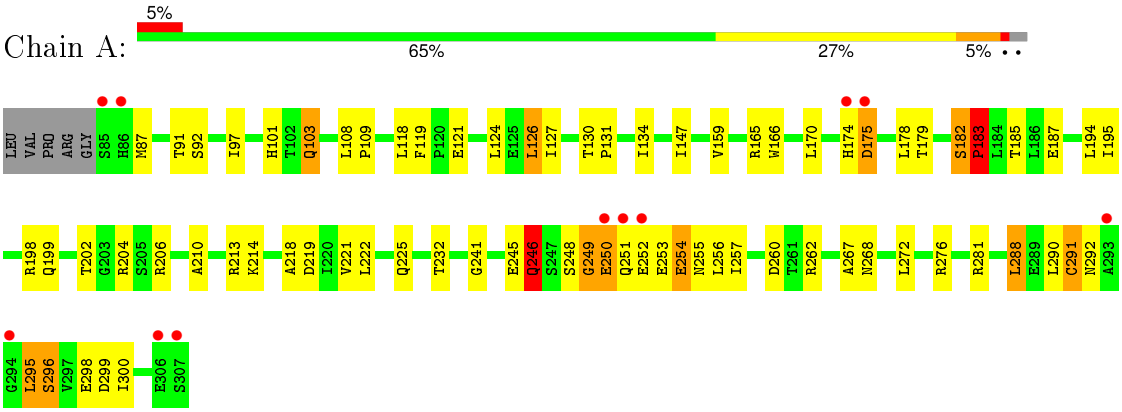
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	138	Total O 138 138	0	0
2	C	88	Total O 88 88	0	0
2	D	62	Total O 62 62	0	0

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.

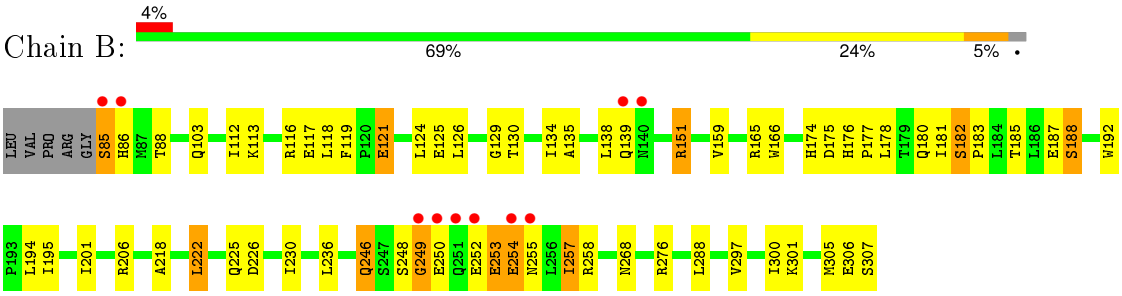
- Molecule 1: HTH-type transcriptional regulator cbl

Chain A:



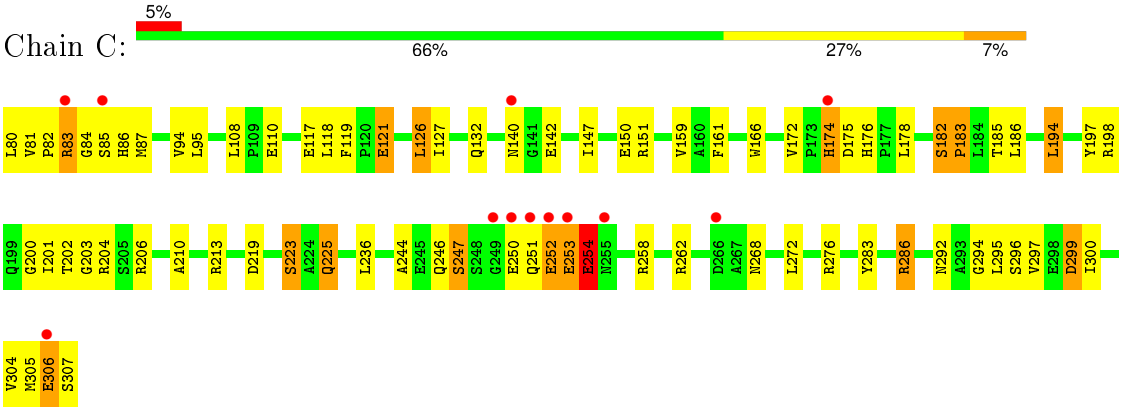
- Molecule 1: HTH-type transcriptional regulator cbl

Chain B:



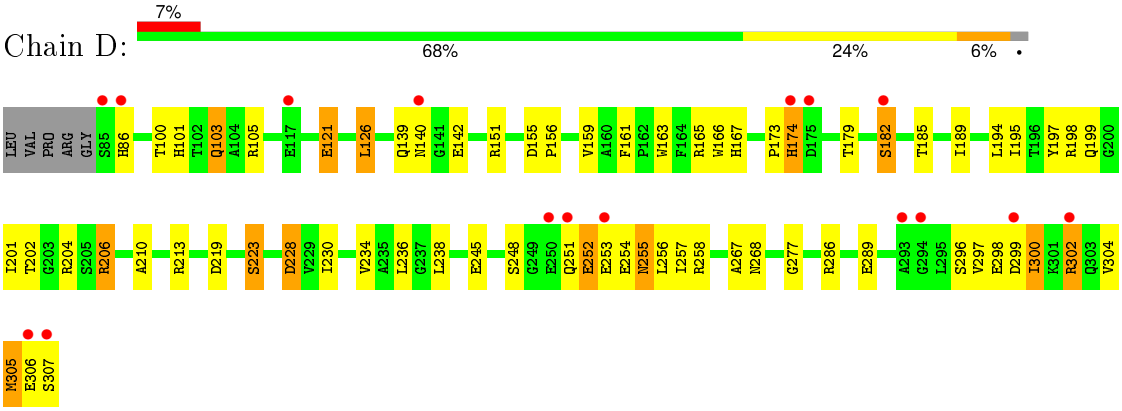
- Molecule 1: HTH-type transcriptional regulator cbl

Chain C:



• Molecule 1: HTH-type transcriptional regulator cbl

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	169.69Å 242.37Å 101.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.80) 99.8 (29.90-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.226 0.186 , 0.183	Depositor DCC
R_{free} test set	2636 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 51751 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

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	0.80	2/1844 (0.1%)	0.91	6/2507 (0.2%)
1	B	0.84	0/1834	0.93	4/2493 (0.2%)
1	C	0.77	0/1871	0.84	2/2544 (0.1%)
1	D	0.70	1/1825 (0.1%)	0.84	4/2481 (0.2%)
All	All	0.78	3/7374 (0.0%)	0.88	16/10025 (0.2%)

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	2
1	C	0	3
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	CYS	CB-SG	-6.44	1.71	1.82
1	A	175	ASP	CB-CG	5.51	1.63	1.51
1	D	307	SER	C-O	5.21	1.33	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	SER	C-N-CD	-11.14	96.10	120.60
1	A	183	PRO	N-CA-C	-8.07	91.13	112.10
1	A	182	SER	C-N-CA	6.63	149.85	122.00
1	D	126	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	222	LEU	CA-CB-CG	6.19	129.53	115.30
1	B	183	PRO	N-CA-C	-5.92	96.72	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	286	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	D	182	SER	C-N-CD	5.56	140.07	128.40
1	D	151	ARG	CB-CA-C	-5.49	99.43	110.40
1	A	246	GLN	CA-CB-CG	-5.29	101.75	113.40
1	A	182	SER	N-CA-C	5.26	125.19	111.00
1	C	126	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	126	LEU	CA-CB-CG	5.21	127.30	115.30
1	B	249	GLY	N-CA-C	-5.13	100.28	113.10
1	B	151	ARG	CB-CA-C	-5.08	100.23	110.40
1	D	126	LEU	CB-CG-CD1	-5.05	102.41	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	SER	Peptide
1	B	182	SER	Mainchain,Peptide
1	C	182	SER	Peptide
1	C	254	GLU	Peptide
1	C	81	VAL	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	1807	0	1802	55	0
1	B	1798	0	1795	55	1
1	C	1834	0	1832	52	2
1	D	1789	0	1779	49	1
2	A	92	0	0	7	1
2	B	138	0	0	6	1
2	C	88	0	0	2	1
2	D	62	0	0	2	0
All	All	7608	0	7208	206	4

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 14.

All (206) 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:B:176:HIS:HD2	1:B:178:LEU:H	1.08	1.02
1:B:246:GLN:C	1:B:248:SER:H	1.67	0.97
1:C:82:PRO:C	1:C:83:ARG:HD2	1.84	0.96
1:A:262:ARG:HD2	2:A:398:HOH:O	1.66	0.95
1:C:176:HIS:HD2	1:C:178:LEU:H	0.99	0.93
1:C:176:HIS:CD2	1:C:178:LEU:H	1.89	0.90
1:A:250:GLU:HG2	2:A:361:HOH:O	1.71	0.90
1:B:176:HIS:CD2	1:B:178:LEU:H	1.90	0.90
1:B:116:ARG:NH1	2:B:704:HOH:O	2.07	0.88
1:B:180[A]:GLN:OE1	2:B:323:HOH:O	1.91	0.87
1:A:225:GLN:HE22	1:B:129:GLY:HA2	1.38	0.87
1:B:121:GLU:OE2	2:B:905:HOH:O	1.94	0.85
1:D:210:ALA:HA	1:D:213:ARG:NH1	1.91	0.85
1:D:305:MET:HE3	1:D:305:MET:HA	1.58	0.84
1:B:250:GLU:HA	1:B:250:GLU:OE1	1.78	0.83
1:C:83:ARG:N	1:C:83:ARG:HD2	1.91	0.81
1:A:292:ASN:HD22	1:A:295:LEU:HD21	1.45	0.80
1:B:181:ILE:O	1:B:182:SER:HB3	1.83	0.79
1:D:305:MET:CE	1:D:305:MET:HA	2.13	0.77
1:D:161:PHE:CE2	1:D:300:ILE:HG22	2.21	0.76
1:B:250:GLU:HG3	1:B:253:GLU:HB2	1.67	0.74
1:B:250:GLU:CG	1:B:253:GLU:HB2	2.16	0.74
1:B:254:GLU:O	1:B:255:ASN:HB2	1.86	0.74
1:D:277:GLY:HA2	1:D:305:MET:HE3	1.71	0.71
1:A:130:THR:O	1:A:134:ILE:HG13	1.91	0.70
1:A:179:THR:HG22	1:A:257[B]:ILE:HD11	1.73	0.69
1:D:210:ALA:HA	1:D:213:ARG:HH11	1.56	0.68
1:A:174[A]:HIS:CD2	1:A:255:ASN:HA	2.29	0.68
1:B:118:LEU:HD23	1:B:119:PHE:CE2	2.29	0.66
1:C:252:GLU:OE1	1:C:254:GLU:HG3	1.94	0.66
1:A:213:ARG:HD2	2:A:395:HOH:O	1.96	0.66
1:B:246:GLN:C	1:B:248:SER:N	2.43	0.64
1:C:201:ILE:HG22	1:C:202:THR:OG1	1.97	0.64
1:B:166:TRP:CG	1:B:246:GLN:NE2	2.66	0.64
1:A:232:THR:O	2:A:363:HOH:O	2.14	0.64
1:D:161:PHE:CD2	1:D:300:ILE:HG22	2.33	0.64
1:A:225:GLN:NE2	1:B:129:GLY:HA2	2.12	0.63
1:C:82:PRO:CA	1:C:83:ARG:HD2	2.28	0.63
1:A:131:PRO:HD2	2:A:340:HOH:O	1.97	0.63
1:C:140:ASN:HB2	1:C:142:GLU:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201[B]:ILE:HD11	2:B:450:HOH:O	1.99	0.62
1:D:121:GLU:HA	1:D:121:GLU:OE1	1.98	0.61
1:D:206:ARG:HD3	1:D:206:ARG:N	2.16	0.61
1:B:135:ALA:O	1:B:139[A]:GLN:HG2	2.00	0.61
1:C:82:PRO:HA	1:C:83:ARG:HD2	1.83	0.61
1:C:306:GLU:OE1	1:C:306:GLU:HA	1.99	0.61
1:C:213:ARG:HD2	2:C:969:HOH:O	2.00	0.61
1:B:112:ILE:HG12	1:B:124:LEU:HD21	1.82	0.60
1:C:176:HIS:HD2	1:C:178:LEU:N	1.84	0.60
1:D:159:VAL:HG11	1:D:304:VAL:HG22	1.83	0.60
1:D:140:ASN:HB2	2:D:627:HOH:O	2.01	0.59
1:A:194:LEU:HD12	1:A:218:ALA:HB1	1.84	0.59
1:C:244:ALA:O	1:C:247:SER:OG	2.19	0.59
1:B:195:ILE:HG22	1:B:230:ILE:HG23	1.85	0.59
1:A:298:GLU:OE1	1:A:298:GLU:N	2.34	0.58
1:B:297:VAL:CG1	1:B:301:LYS:HE3	2.34	0.58
1:D:185:THR:O	1:D:189:ILE:HG13	2.02	0.58
1:C:118:LEU:HD23	1:C:119:PHE:CE2	2.38	0.58
1:D:142:GLU:HG3	2:D:627:HOH:O	2.03	0.58
1:A:103:GLN:HG3	1:A:147:ILE:HG22	1.85	0.58
1:C:305:MET:O	1:C:307:SER:N	2.37	0.58
1:B:116:ARG:NE	2:B:992:HOH:O	2.26	0.58
1:D:252:GLU:HG2	1:D:254:GLU:HG3	1.84	0.58
1:A:210:ALA:HA	1:A:213:ARG:NH1	2.20	0.57
1:A:206:ARG:NH1	1:A:267:ALA:O	2.37	0.57
1:B:176:HIS:HD2	1:B:178:LEU:N	1.91	0.57
1:C:110:GLU:HA	1:C:110:GLU:OE1	2.03	0.57
1:B:201[A]:ILE:HD11	1:B:225:GLN:HA	1.87	0.57
1:D:198:ARG:HG2	1:D:223:SER:HB3	1.85	0.56
1:A:183:PRO:HD2	1:A:183:PRO:O	2.05	0.56
1:B:86:HIS:HD2	1:B:88:THR:OG1	1.88	0.56
1:A:179:THR:CG2	1:A:257[B]:ILE:HD11	2.35	0.56
1:A:195:ILE:HG23	1:A:222:LEU:HB3	1.87	0.56
1:D:297:VAL:HA	1:D:300:ILE:HD11	1.88	0.55
1:B:166:TRP:CD2	1:B:246:GLN:NE2	2.75	0.55
1:C:297:VAL:HA	1:C:300:ILE:HD12	1.88	0.55
1:C:198:ARG:HG2	1:C:223:SER:HB3	1.89	0.55
1:D:277:GLY:HA2	1:D:305:MET:CE	2.37	0.55
1:D:173:PRO:HA	1:D:256:LEU:HD23	1.88	0.54
1:C:210:ALA:HA	1:C:213:ARG:NH1	2.22	0.54
1:D:230:ILE:O	1:D:234:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187[A]:GLU:CD	1:A:187[A]:GLU:H	2.12	0.53
1:A:251:GLN:O	1:A:251:GLN:HG2	2.08	0.53
1:A:292:ASN:HD22	1:A:295:LEU:CD2	2.19	0.52
1:D:101:HIS:CE1	1:D:105:ARG:HG3	2.44	0.52
1:A:296:SER:HB3	1:A:299:ASP:OD2	2.11	0.51
1:B:249:GLY:HA3	1:B:258:ARG:HD3	1.92	0.51
1:D:165:ARG:NH2	1:D:267:ALA:HB3	2.25	0.51
1:D:298[B]:GLU:H	1:D:298[B]:GLU:CD	2.14	0.50
1:C:166:TRP:CE2	1:C:268:ASN:HB2	2.46	0.50
1:A:118:LEU:HD23	1:A:119:PHE:CE2	2.46	0.50
1:B:194:LEU:HD23	1:B:218:ALA:HB1	1.93	0.50
1:B:113:LYS:O	1:B:117:GLU:HG2	2.11	0.50
1:A:166:TRP:CE2	1:A:268:ASN:HB2	2.46	0.50
1:D:298[B]:GLU:N	1:D:298[B]:GLU:CD	2.65	0.50
1:A:183:PRO:CD	1:A:183:PRO:O	2.55	0.50
1:C:252:GLU:C	1:C:253:GLU:HG3	2.31	0.50
1:A:281:ARG:CZ	1:D:219:ASP:HB2	2.42	0.50
1:A:248:SER:O	1:A:249:GLY:C	2.50	0.50
1:D:139:GLN:HG3	1:D:140:ASN:ND2	2.27	0.49
1:C:147:ILE:HG12	1:C:272:LEU:HD23	1.94	0.49
1:B:250:GLU:HG2	1:B:253:GLU:HB2	1.93	0.49
1:A:245:GLU:OE2	1:A:262:ARG:NH2	2.46	0.49
1:C:194:LEU:HB2	1:C:219:ASP:O	2.13	0.48
1:C:306:GLU:OE1	1:C:306:GLU:CA	2.62	0.48
1:B:165:ARG:HA	1:B:268:ASN:O	2.13	0.48
1:D:253:GLU:O	1:D:254:GLU:CG	2.62	0.48
1:A:185:THR:HB	1:A:187[A]:GLU:OE1	2.13	0.48
1:A:253:GLU:CD	1:A:253:GLU:H	2.17	0.48
1:D:100:THR:OG1	1:D:103:GLN:NE2	2.47	0.47
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.70	0.47
1:D:286:ARG:HD3	1:D:289:GLU:OE2	2.15	0.46
1:D:297:VAL:HG12	1:D:298[B]:GLU:OE2	2.16	0.46
1:D:161:PHE:CZ	1:D:300:ILE:HG22	2.50	0.46
1:C:110:GLU:OE1	1:C:110:GLU:CA	2.63	0.46
1:A:288:LEU:O	1:A:291:CYS:HB2	2.15	0.46
1:C:251:GLN:HG3	1:C:251:GLN:O	2.15	0.46
1:A:214:LYS:NZ	2:A:367:HOH:O	2.49	0.46
1:C:82:PRO:HD2	1:C:117:GLU:OE1	2.16	0.46
1:D:195:ILE:HD11	1:D:238:LEU:HB3	1.98	0.46
1:B:236:LEU:O	1:B:236:LEU:HG	2.14	0.46
1:C:150:GLU:HG3	1:C:200:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ARG:NH1	1:D:228:ASP:OD2	2.48	0.45
1:B:206:ARG:HG3	1:B:268:ASN:OD1	2.16	0.45
1:B:257:ILE:HD13	1:B:257:ILE:HG23	1.60	0.45
1:A:254:GLU:HB2	1:A:255:ASN:ND2	2.31	0.45
1:A:292:ASN:HB3	1:A:295:LEU:HG	1.98	0.45
1:C:295:LEU:HB3	1:C:300:ILE:HD11	1.97	0.45
1:C:296:SER:O	1:C:299:ASP:HB2	2.17	0.45
1:C:85:SER:HB3	2:C:622:HOH:O	2.16	0.45
1:B:166:TRP:HB2	1:B:246:GLN:HE21	1.82	0.45
1:A:281:ARG:HD3	2:A:366:HOH:O	2.17	0.45
1:C:201:ILE:O	1:C:202:THR:C	2.56	0.45
1:B:85:SER:HB3	1:B:86:HIS:ND1	2.32	0.45
1:B:181:ILE:HG23	1:B:181:ILE:HD12	1.63	0.45
1:B:177:PRO:HG2	1:B:192:TRP:HH2	1.82	0.45
1:A:147:ILE:HG12	1:A:272:LEU:HD23	1.97	0.45
1:D:255:ASN:H	1:D:256:LEU:HG	1.82	0.45
1:D:195:ILE:HG22	1:D:230:ILE:HG23	1.99	0.44
1:A:295:LEU:HB2	1:A:300:ILE:HD11	1.99	0.44
1:A:108:LEU:N	1:A:109:PRO:CD	2.81	0.44
1:A:166:TRP:CD2	1:A:246:GLN:NE2	2.86	0.44
1:C:194:LEU:HA	1:C:194:LEU:HD13	1.64	0.44
1:B:246:GLN:H	1:B:246:GLN:HG3	0.88	0.44
1:A:97:ILE:HD12	1:A:124:LEU:HD11	2.00	0.44
1:C:185[B]:THR:OG1	1:C:186:LEU:N	2.51	0.43
1:A:101:HIS:HD2	1:B:226:ASP:OD1	2.01	0.43
1:B:85:SER:HB3	1:B:86:HIS:H	1.48	0.43
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.75	0.43
1:C:198:ARG:HH21	1:C:225:GLN:NE2	2.16	0.43
1:D:236:LEU:O	1:D:236:LEU:HG	2.17	0.43
1:D:165:ARG:HH21	1:D:267:ALA:HB3	1.83	0.43
1:A:281:ARG:NH2	1:D:219:ASP:HB2	2.32	0.43
1:D:166:TRP:CE2	1:D:268:ASN:HB2	2.53	0.43
1:D:305:MET:CE	1:D:305:MET:CA	2.88	0.43
1:D:296:SER:O	1:D:300:ILE:HG12	2.19	0.43
1:D:167:HIS:O	1:D:245:GLU:HG2	2.18	0.43
1:B:194:LEU:HD12	1:B:195:ILE:N	2.33	0.43
1:C:292:ASN:OD1	1:C:294:GLY:N	2.37	0.43
1:B:124:LEU:HD12	1:B:125:GLU:N	2.33	0.43
1:C:132[B]:GLN:HE21	1:C:151:ARG:CZ	2.32	0.43
1:B:112:ILE:O	1:B:116:ARG:HG2	2.19	0.42
1:A:214:LYS:HD3	1:A:214:LYS:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:MET:O	1:B:306:GLU:C	2.58	0.42
1:C:197:TYR:O	1:C:204:ARG:HD3	2.19	0.42
1:A:219:ASP:C	1:A:219:ASP:OD1	2.58	0.42
1:B:246:GLN:O	1:B:248:SER:N	2.49	0.42
1:A:199:GLN:HA	1:A:204:ARG:HG2	2.00	0.42
1:C:172:VAL:HG13	1:C:176:HIS:HB3	2.02	0.42
1:A:174[B]:HIS:CD2	1:A:175:ASP:OD1	2.73	0.42
1:B:195:ILE:CG2	1:B:230:ILE:HG23	2.49	0.42
1:D:197:TYR:O	1:D:204:ARG:HD3	2.18	0.42
1:C:247:SER:HB2	1:C:258:ARG:HH22	1.85	0.42
1:C:203:GLY:O	1:C:204:ARG:C	2.57	0.42
1:B:175:ASP:HB3	2:B:936:HOH:O	2.20	0.42
1:D:248:SER:HB3	1:D:258:ARG:CZ	2.50	0.42
1:D:163:TRP:CD1	1:D:163:TRP:C	2.89	0.42
1:A:159:VAL:HG22	1:A:276:ARG:CZ	2.50	0.42
1:C:132[B]:GLN:HE21	1:C:151:ARG:NH2	2.17	0.41
1:B:288:LEU:HD12	1:B:300:ILE:HD13	2.02	0.41
1:A:91:THR:O	1:A:121:GLU:HB2	2.21	0.41
1:D:299:ASP:OD1	1:D:302:ARG:NH1	2.53	0.41
1:C:83:ARG:O	1:C:86:HIS:NE2	2.53	0.41
1:A:253:GLU:CB	1:A:256:LEU:HB2	2.51	0.41
1:B:174:HIS:HA	1:B:257:ILE:HG21	2.03	0.41
1:C:159:VAL:HG22	1:C:276:ARG:CZ	2.50	0.41
1:C:296:SER:HB3	1:C:299:ASP:HB2	2.03	0.41
1:B:185:THR:O	1:B:188:SER:HB2	2.21	0.41
1:D:155:ASP:HA	1:D:156:PRO:HD2	1.83	0.41
1:C:161:PHE:CZ	1:C:300:ILE:HG23	2.56	0.41
1:B:130:THR:O	1:B:134:ILE:HG13	2.19	0.41
1:A:170:LEU:HD12	1:A:241:GLY:O	2.21	0.41
1:A:260:ASP:OD1	1:A:260:ASP:C	2.59	0.41
1:C:304:VAL:HG12	1:C:305:MET:CE	2.51	0.41
1:A:253:GLU:HB2	1:A:256:LEU:HB2	2.03	0.41
1:D:159:VAL:CG1	1:D:304:VAL:HG22	2.49	0.40
1:C:183:PRO:HD2	1:C:183:PRO:O	2.21	0.40
1:A:292:ASN:ND2	1:A:295:LEU:HD21	2.25	0.40
1:B:159:VAL:HG22	1:B:276:ARG:CZ	2.51	0.40
1:C:95:LEU:HB2	1:C:283:TYR:CE2	2.57	0.40
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.94	0.40
1:B:166:TRP:CE2	1:B:268:ASN:HB2	2.57	0.40
1:D:253:GLU:O	1:D:254:GLU:HG2	2.21	0.40
1:C:304:VAL:HG12	1:C:305:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:CD	1:D:289:GLU:OE2	2.69	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:OE2	2:B:905:HOH:O[3_555]	1.90	0.30
1:D:179:THR:O	1:D:182:SER:CB[3_655]	2.11	0.09
2:A:328:HOH:O	2:C:705:HOH:O[3_555]	2.15	0.05
1:B:187:GLU:OE1	1:C:83:ARG:NH2[8_555]	2.18	0.02

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	225/228 (99%)	215 (96%)	7 (3%)	3 (1%)	15 44
1	B	224/228 (98%)	206 (92%)	17 (8%)	1 (0%)	39 74
1	C	229/228 (100%)	210 (92%)	14 (6%)	5 (2%)	8 28
1	D	223/228 (98%)	216 (97%)	5 (2%)	2 (1%)	21 55
All	All	901/912 (99%)	847 (94%)	43 (5%)	11 (1%)	16 47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	249	GLY
1	C	84	GLY
1	D	306	GLU
1	A	202	THR
1	D	174	HIS

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Mol	Chain	Res	Type
1	B	253	GLU
1	C	183	PRO
1	C	250	GLU
1	C	174	HIS
1	C	254	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	197/197 (100%)	181 (92%)	16 (8%)	15 39
1	B	196/197 (100%)	184 (94%)	12 (6%)	23 55
1	C	200/197 (102%)	177 (88%)	23 (12%)	7 21
1	D	195/197 (99%)	176 (90%)	19 (10%)	10 29
All	All	788/788 (100%)	718 (91%)	70 (9%)	12 34

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	MET
1	A	92	SER
1	A	103	GLN
1	A	126	LEU
1	A	127	ILE
1	A	165	ARG
1	A	198	ARG
1	A	221	VAL
1	A	246	GLN
1	A	250	GLU
1	A	252	GLU
1	A	254	GLU
1	A	288	LEU
1	A	290	LEU
1	A	295	LEU
1	A	296	SER

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Mol	Chain	Res	Type
1	B	85	SER
1	B	103	GLN
1	B	121	GLU
1	B	126	LEU
1	B	151	ARG
1	B	188	SER
1	B	222	LEU
1	B	246	GLN
1	B	252	GLU
1	B	254	GLU
1	B	257	ILE
1	B	307	SER
1	C	80	LEU
1	C	83	ARG
1	C	87	MET
1	C	94	VAL
1	C	121	GLU
1	C	126	LEU
1	C	127	ILE
1	C	174	HIS
1	C	175	ASP
1	C	182	SER
1	C	194	LEU
1	C	206	ARG
1	C	223	SER
1	C	225	GLN
1	C	236	LEU
1	C	246	GLN
1	C	247	SER
1	C	252	GLU
1	C	253	GLU
1	C	262	ARG
1	C	286	ARG
1	C	299	ASP
1	C	306	GLU
1	D	86	HIS
1	D	103	GLN
1	D	121	GLU
1	D	126	LEU
1	D	174	HIS
1	D	194	LEU
1	D	199	GLN

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Mol	Chain	Res	Type
1	D	201	ILE
1	D	202	THR
1	D	206	ARG
1	D	223	SER
1	D	228	ASP
1	D	251	GLN
1	D	252	GLU
1	D	255	ASN
1	D	257	ILE
1	D	300	ILE
1	D	302	ARG
1	D	305	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	225	GLN
1	A	255	ASN
1	A	292	ASN
1	B	103	GLN
1	B	176	HIS
1	B	225	GLN
1	C	176	HIS
1	C	225	GLN
1	D	103	GLN
1	D	140	ASN
1	D	157	GLN
1	D	255	ASN

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

There are no ligands in this entry.

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	223/228 (97%)	-0.18	11 (4%)	33	22	22, 36, 57, 87	6 (2%)
1	B	223/228 (97%)	-0.32	10 (4%)	37	26	23, 36, 68, 94	8 (3%)
1	C	228/228 (100%)	-0.13	12 (5%)	30	20	23, 37, 70, 94	6 (2%)
1	D	223/228 (97%)	-0.12	16 (7%)	18	10	25, 37, 61, 81	6 (2%)
All	All	897/912 (98%)	-0.19	49 (5%)	29	18	22, 37, 67, 94	26 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	GLN	6.8
1	D	251	GLN	6.6
1	D	85	SER	6.1
1	C	252	GLU	5.4
1	C	250	GLU	5.3
1	B	250	GLU	5.1
1	D	253	GLU	4.7
1	A	251	GLN	4.7
1	B	85	SER	4.6
1	D	250	GLU	4.6
1	C	253	GLU	4.3
1	D	307	SER	4.2
1	D	175[A]	ASP	4.2
1	B	86	HIS	4.2
1	D	86	HIS	4.0
1	C	249	GLY	3.7
1	A	174[A]	HIS	3.4
1	A	307	SER	3.4
1	D	174	HIS	3.4
1	A	250	GLU	3.2
1	B	255	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	SER	3.1
1	C	140	ASN	3.1
1	D	302	ARG	3.0
1	C	174	HIS	2.9
1	D	306	GLU	2.9
1	A	86	HIS	2.8
1	A	175	ASP	2.7
1	C	306	GLU	2.7
1	B	252	GLU	2.6
1	B	251	GLN	2.5
1	D	182	SER	2.5
1	B	140	ASN	2.5
1	A	294	GLY	2.5
1	B	254	GLU	2.5
1	D	140	ASN	2.4
1	D	117	GLU	2.4
1	C	83	ARG	2.3
1	C	255	ASN	2.3
1	A	252	GLU	2.3
1	B	249	GLY	2.2
1	D	294	GLY	2.2
1	A	306	GLU	2.2
1	A	293	ALA	2.2
1	D	293	ALA	2.2
1	B	139[A]	GLN	2.1
1	C	266	ASP	2.1
1	D	299	ASP	2.1
1	C	85	SER	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.