Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:08 AM GMT

PDB ID	:	3H8A
Title	:	Crystal structure of E. coli enolase bound to its cognate RNase E recognition domain
Authors	:	Nurmohamed, S.; Luisi, B.F.
Deposited on	:	2009-04-29
Resolution	:	1.90 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:

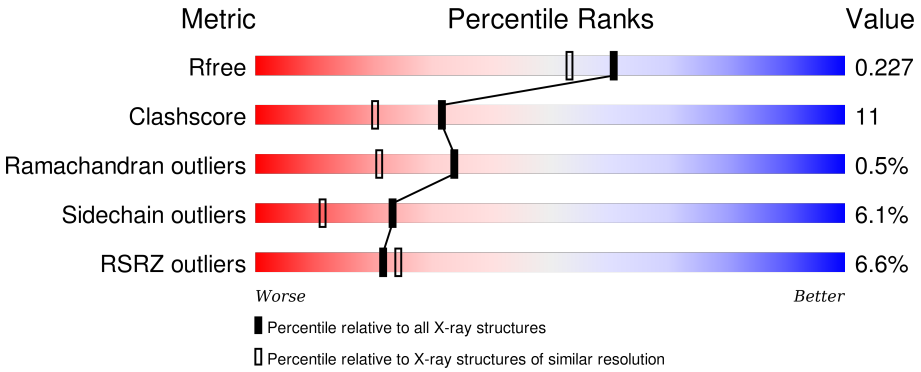
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	432	87% 11%
1	B	432	6% 79% 18%
1	C	432	12% 81% 15%
1	D	432	5% 84% 14%
2	E	28	14% 64% 32%

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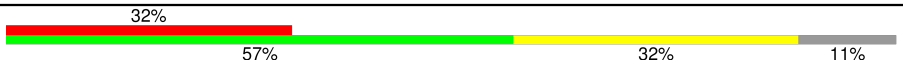
Mol	Chain	Length	Quality of chain
2	F	28	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14368 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3187	2000	544	630	13			
1	B	430	Total	C	N	O	S	0	0	0
			3178	1992	541	632	13			
1	C	430	Total	C	N	O	S	0	0	0
			3186	1997	544	632	13			
1	D	431	Total	C	N	O	S	0	0	0
			3163	1980	541	629	13			

- Molecule 2 is a protein called RNase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	28	Total	C	N	O	S	0	0	0
			213	139	37	36	1			
2	F	25	Total	C	N	O	S	0	0	0
			187	122	31	33	1			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	382	Total	O	0	0
			382	382		
4	B	268	Total	O	0	0
			268	268		

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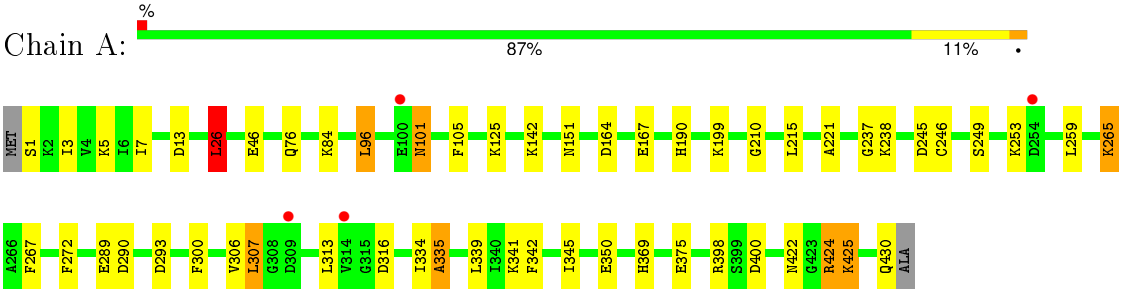
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	247	Total O 247 247	0	0
4	D	293	Total O 293 293	0	0
4	E	34	Total O 34 34	0	0
4	F	28	Total O 28 28	0	0

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.

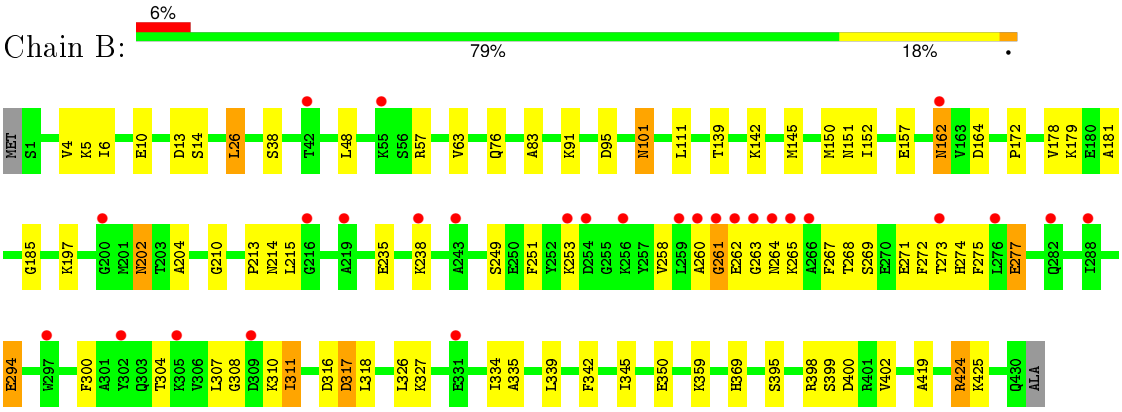
- Molecule 1: Enolase

Chain A:



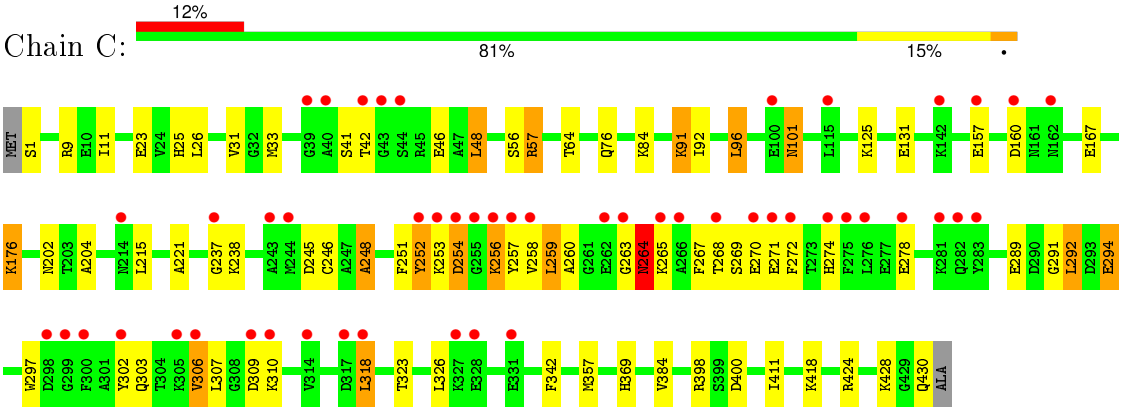
- Molecule 1: Enolase

Chain B:



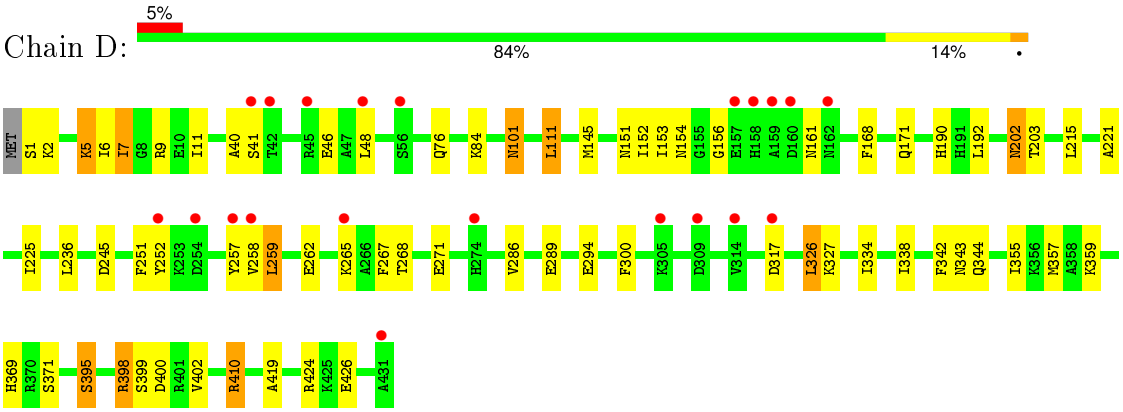
- Molecule 1: Enolase

Chain C:



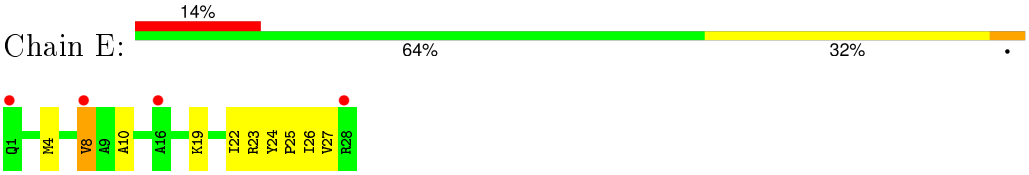
- Molecule 1: Enolase

Chain D:



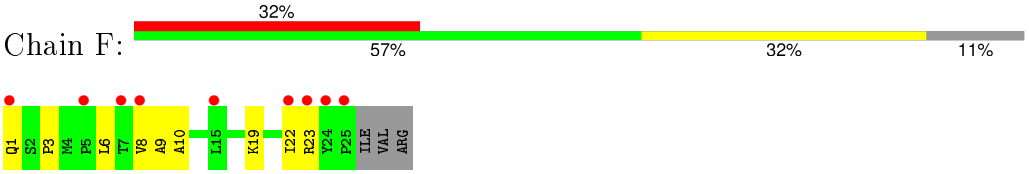
- Molecule 2: RNase E

Chain E:



- Molecule 2: RNase E

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.88Å 110.21Å 160.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 1.90 24.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.89-1.90) 99.0 (24.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.226 0.183 , 0.227	Depositor DCC
R_{free} test set	7214 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 144179 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14368	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: MG

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	0.95	2/3232 (0.1%)	0.76	3/4354 (0.1%)
1	B	0.90	2/3220 (0.1%)	0.77	2/4340 (0.0%)
1	C	0.94	4/3228 (0.1%)	0.79	1/4348 (0.0%)
1	D	0.96	3/3204 (0.1%)	0.76	4/4322 (0.1%)
2	E	0.94	0/219	0.64	0/300
2	F	1.09	0/193	0.76	0/265
All	All	0.94	11/13296 (0.1%)	0.77	10/17929 (0.1%)

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	D	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	CYS	CB-SG	-6.56	1.71	1.82
1	C	246	CYS	CB-SG	-6.20	1.71	1.82
1	D	426	GLU	CD-OE2	-5.71	1.19	1.25
1	C	131	GLU	CD-OE2	-5.66	1.19	1.25
1	B	395	SER	CB-OG	-5.57	1.35	1.42
1	C	252	TYR	CD2-CE2	-5.36	1.31	1.39
1	D	395	SER	CB-OG	-5.30	1.35	1.42
1	A	46	GLU	CD-OE2	-5.26	1.19	1.25
1	D	426	GLU	CD-OE1	-5.26	1.19	1.25
1	B	14	SER	CB-OG	-5.14	1.35	1.42
1	C	131	GLU	CD-OE1	-5.05	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	161	ASN	N-CA-CB	8.21	125.37	110.60
1	B	13	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	A	13	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	160	ASP	N-CA-C	-5.74	95.51	111.00
1	A	26	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	424	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	57	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	410	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	161	ASN	N-CA-C	-5.09	97.24	111.00
1	D	111	LEU	CB-CG-CD2	5.08	119.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156	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	3187	0	3212	32	0
1	B	3178	0	3180	69	0
1	C	3186	0	3205	82	0
1	D	3163	0	3152	90	0
2	E	213	0	227	12	0
2	F	187	0	194	21	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	382	0	0	5	0
4	B	268	0	0	6	0
4	C	247	0	0	9	0
4	D	293	0	0	10	0
4	E	34	0	0	2	0
4	F	28	0	0	3	0
All	All	14368	0	13170	280	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 11.

All (280) 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:268:THR:CG2	1:B:271:GLU:HG3	1.35	1.54
1:C:33:MET:CE	2:F:9:ALA:HB3	1.58	1.31
1:C:302:TYR:O	1:C:306:VAL:HG23	1.39	1.22
1:B:268:THR:HG22	1:B:271:GLU:CG	1.73	1.17
1:D:5:LYS:HZ1	2:F:23:ARG:CD	1.62	1.12
1:C:33:MET:HE3	2:F:9:ALA:HB3	1.22	1.12
1:C:259:LEU:HD23	1:C:259:LEU:N	1.63	1.09
1:B:268:THR:CG2	1:B:271:GLU:CG	2.30	1.07
1:C:326:LEU:HD23	1:C:357:MET:HE3	1.26	1.07
1:C:33:MET:HE3	2:F:9:ALA:CB	1.87	1.02
1:D:327:LYS:CB	1:D:357:MET:HE1	1.89	1.02
1:C:33:MET:HE2	2:F:9:ALA:HB3	1.40	1.01
1:D:327:LYS:HA	1:D:357:MET:HE2	1.40	1.00
1:B:268:THR:HG23	1:B:271:GLU:H	1.24	1.00
1:B:268:THR:HG22	1:B:271:GLU:HG3	0.99	0.99
1:D:101:ASN:HD22	1:D:101:ASN:H	1.02	0.97
1:C:259:LEU:CD2	1:C:259:LEU:N	2.30	0.95
1:C:33:MET:CE	2:F:9:ALA:CB	2.42	0.93
1:C:323:THR:HG22	1:C:357:MET:HE2	1.52	0.92
1:C:258:VAL:C	1:C:259:LEU:HD23	1.89	0.92
1:B:5:LYS:HZ1	2:E:23:ARG:HG3	1.34	0.91
1:D:152:ILE:HG13	4:D:737:HOH:O	1.71	0.89
1:B:5:LYS:NZ	2:E:23:ARG:HG3	1.87	0.89
1:A:422:ASN:HB3	1:A:425:LYS:HD3	1.54	0.89
1:D:327:LYS:CA	1:D:357:MET:CE	2.51	0.88
1:D:5:LYS:HE2	1:D:7:ILE:HD11	1.53	0.88
1:D:327:LYS:HA	1:D:357:MET:CE	2.03	0.88
1:D:5:LYS:CD	1:D:7:ILE:HD11	2.04	0.86
1:D:268:THR:HG23	1:D:271:GLU:H	1.41	0.86
1:B:268:THR:HG21	1:B:271:GLU:HG3	1.53	0.85
1:D:399:SER:HA	1:D:402:VAL:HG22	1.58	0.84
1:D:5:LYS:HZ1	2:F:23:ARG:HD2	1.39	0.84
1:D:5:LYS:HB3	1:D:5:LYS:HZ3	1.42	0.84
1:D:252:TYR:CD1	1:D:257:TYR:CE1	2.65	0.83
1:C:270:GLU:O	1:C:274:HIS:HD2	1.60	0.83
1:D:101:ASN:HB3	4:D:613:HOH:O	1.79	0.83
1:B:277:GLU:HG3	1:B:307:LEU:HD21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LYS:CE	1:D:7:ILE:HD11	2.09	0.82
1:C:270:GLU:O	1:C:274:HIS:CD2	2.32	0.82
1:D:327:LYS:CA	1:D:357:MET:HE2	2.09	0.81
1:D:5:LYS:NZ	2:F:23:ARG:CD	2.43	0.81
1:D:327:LYS:CB	1:D:357:MET:CE	2.59	0.81
1:B:268:THR:HG23	1:B:271:GLU:HG3	1.59	0.80
1:C:424:ARG:HH11	1:C:430:GLN:NE2	1.79	0.80
1:C:91:LYS:HD3	4:C:902:HOH:O	1.81	0.79
1:D:101:ASN:H	1:D:101:ASN:ND2	1.80	0.79
1:D:268:THR:HG22	1:D:271:GLU:HB2	1.64	0.78
1:B:263:GLY:O	1:B:264:ASN:HB3	1.84	0.78
1:D:101:ASN:HD22	1:D:101:ASN:N	1.81	0.78
1:D:252:TYR:CD1	1:D:257:TYR:CZ	2.72	0.78
1:C:323:THR:HA	1:C:357:MET:HE1	1.67	0.77
1:D:5:LYS:NZ	2:F:23:ARG:NE	2.35	0.75
1:C:326:LEU:HB3	1:C:357:MET:HE1	1.71	0.72
1:B:76:GLN:HE22	1:D:6:ILE:H	1.38	0.72
1:C:310:LYS:HG3	4:C:1265:HOH:O	1.90	0.72
1:D:327:LYS:CA	1:D:357:MET:HE1	2.16	0.71
1:C:31:VAL:HG11	2:F:6:LEU:HD12	1.73	0.70
1:C:323:THR:HA	1:C:357:MET:CE	2.21	0.70
1:B:6:ILE:H	1:D:76:GLN:HE22	1.39	0.70
1:D:5:LYS:HD2	1:D:7:ILE:CD1	2.22	0.70
1:B:277:GLU:CG	1:B:307:LEU:HD21	2.21	0.70
1:D:5:LYS:HZ1	2:F:23:ARG:NE	1.88	0.69
1:C:326:LEU:CD2	1:C:357:MET:HE3	2.12	0.69
1:C:91:LYS:HZ3	1:C:91:LYS:HA	1.57	0.69
1:D:268:THR:HG22	1:D:271:GLU:CB	2.22	0.68
1:C:424:ARG:NH1	1:C:430:GLN:NE2	2.41	0.68
1:D:5:LYS:NZ	1:D:5:LYS:HB3	2.08	0.68
1:B:5:LYS:HD2	4:D:456:HOH:O	1.93	0.68
1:D:1:SER:OG	1:D:84:LYS:HD2	1.93	0.68
1:C:302:TYR:O	1:C:306:VAL:CG2	2.30	0.68
1:C:258:VAL:C	1:C:259:LEU:CD2	2.59	0.67
1:B:202:ASN:ND2	1:B:204:ALA:H	1.91	0.67
1:C:176:LYS:HE2	1:C:176:LYS:HA	1.75	0.67
1:D:5:LYS:CD	1:D:7:ILE:CD1	2.72	0.67
1:C:33:MET:HE2	2:F:9:ALA:CB	2.18	0.66
1:A:1:SER:OG	1:A:84:LYS:HE3	1.96	0.66
1:B:399:SER:HA	1:B:402:VAL:HG22	1.77	0.66
1:B:264:ASN:O	1:B:264:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLY:O	1:C:265:LYS:N	2.30	0.65
1:C:91:LYS:HE3	4:C:902:HOH:O	1.96	0.64
1:D:268:THR:HG22	1:D:271:GLU:CG	2.28	0.64
1:C:252:TYR:CD1	1:C:257:TYR:CE1	2.86	0.64
1:B:268:THR:HG22	1:B:271:GLU:CD	2.17	0.64
1:B:310:LYS:HB2	1:B:311:ILE:HD12	1.79	0.63
1:A:306:VAL:HG12	1:A:307:LEU:HD13	1.80	0.63
1:D:5:LYS:NZ	1:D:5:LYS:CB	2.61	0.63
1:C:326:LEU:HB3	1:C:357:MET:CE	2.29	0.62
1:C:91:LYS:CA	1:C:91:LYS:HZ3	2.12	0.62
1:D:259:LEU:HB3	1:D:262:GLU:HB2	1.83	0.61
1:A:5:LYS:HE2	1:A:7:ILE:HD11	1.83	0.61
1:C:318:LEU:C	1:C:318:LEU:HD12	2.21	0.61
1:C:318:LEU:HD12	1:C:318:LEU:O	2.01	0.60
1:C:91:LYS:HZ3	1:C:91:LYS:CB	2.14	0.60
1:B:6:ILE:H	1:D:76:GLN:NE2	1.99	0.60
1:C:259:LEU:HD11	1:C:272:PHE:HE1	1.66	0.60
1:B:235:GLU:HG3	1:B:238:LYS:HB3	1.84	0.59
1:A:265:LYS:HD2	1:A:267:PHE:CZ	2.36	0.59
1:D:252:TYR:HD1	1:D:257:TYR:CE1	2.21	0.58
1:C:424:ARG:HH11	1:C:430:GLN:HE21	1.49	0.58
1:B:260:ALA:O	1:B:262:GLU:N	2.37	0.58
1:D:268:THR:HG23	1:D:271:GLU:N	2.17	0.58
4:C:436:HOH:O	1:D:402:VAL:HG23	2.03	0.58
1:A:151:ASN:ND2	1:A:210:GLY:HA3	2.19	0.57
1:A:345:ILE:HG12	1:A:350:GLU:HB3	1.86	0.57
1:D:268:THR:CG2	1:D:271:GLU:H	2.14	0.57
1:A:345:ILE:HD13	4:A:509:HOH:O	2.05	0.57
1:D:251:PHE:O	1:D:257:TYR:HA	2.05	0.57
1:C:263:GLY:C	1:C:265:LYS:N	2.58	0.56
1:C:294:GLU:CD	1:C:294:GLU:C	2.64	0.56
1:C:257:TYR:O	1:C:267:PHE:HB2	2.04	0.56
1:D:265:LYS:HG2	1:D:267:PHE:CE1	2.40	0.56
2:F:8:VAL:HG12	4:F:899:HOH:O	2.05	0.56
1:B:76:GLN:NE2	1:D:6:ILE:H	2.05	0.56
1:C:46:GLU:O	1:C:48:LEU:HD13	2.06	0.55
1:B:5:LYS:NZ	4:B:1228:HOH:O	2.39	0.55
2:E:10:ALA:HA	4:E:1233:HOH:O	2.07	0.54
1:D:251:PHE:HB2	1:D:258:VAL:O	2.08	0.54
1:B:202:ASN:HD21	1:B:204:ALA:HB3	1.72	0.54
1:C:91:LYS:CE	4:C:902:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ILE:HG22	1:D:359:LYS:HD2	1.89	0.54
1:D:152:ILE:HG23	1:D:153:ILE:HG12	1.90	0.54
1:D:190:HIS:HD2	4:D:479:HOH:O	1.91	0.54
1:D:5:LYS:HD3	4:D:750:HOH:O	2.07	0.53
1:D:268:THR:HG22	1:D:271:GLU:CD	2.28	0.53
1:B:251:PHE:HB2	1:B:258:VAL:O	2.09	0.53
2:F:3:PRO:HG2	2:F:22:ILE:HD13	1.91	0.53
1:C:263:GLY:C	1:C:265:LYS:H	2.12	0.53
1:B:268:THR:CG2	1:B:271:GLU:H	2.10	0.53
1:B:267:PHE:N	1:B:267:PHE:CD1	2.76	0.53
1:C:23:GLU:OE2	1:C:25:HIS:HE1	1.92	0.53
1:D:7:ILE:N	1:D:7:ILE:HD13	2.24	0.52
1:C:91:LYS:CB	1:C:91:LYS:NZ	2.61	0.52
1:C:310:LYS:CG	4:C:1265:HOH:O	2.52	0.52
1:B:101:ASN:H	1:B:101:ASN:HD22	1.58	0.52
1:C:202:ASN:HD21	1:C:204:ALA:HB3	1.75	0.52
1:B:317:ASP:CG	4:B:1062:HOH:O	2.48	0.51
1:B:164:ASP:OD2	1:B:261:GLY:HA3	2.09	0.51
2:E:23:ARG:O	2:E:26:ILE:HD13	2.10	0.51
1:D:424:ARG:HD2	4:D:653:HOH:O	2.09	0.51
1:D:252:TYR:CE1	1:D:257:TYR:CZ	2.97	0.51
1:C:251:PHE:CD2	1:C:251:PHE:N	2.78	0.51
1:A:339:LEU:HD23	1:A:341:LYS:HE3	1.92	0.51
2:E:22:ILE:CG2	2:E:26:ILE:HD11	2.42	0.50
1:C:167:GLU:HG2	1:C:245:ASP:HB3	1.93	0.50
1:D:399:SER:HA	1:D:402:VAL:CG2	2.37	0.50
1:B:263:GLY:O	1:B:264:ASN:CB	2.52	0.50
1:B:162:ASN:ND2	1:B:261:GLY:HA2	2.26	0.50
1:C:245:ASP:HA	1:C:289:GLU:HB3	1.94	0.50
2:F:10:ALA:HA	4:F:511:HOH:O	2.12	0.50
1:C:76:GLN:NE2	4:C:579:HOH:O	2.45	0.50
1:C:268:THR:H	1:C:271:GLU:HB2	1.76	0.49
1:B:179:LYS:NZ	4:B:778:HOH:O	2.43	0.49
1:B:294:GLU:HB3	1:B:318:LEU:HA	1.94	0.49
1:D:252:TYR:HD1	1:D:257:TYR:CD1	2.30	0.49
1:C:101:ASN:H	1:C:101:ASN:HD22	1.60	0.49
1:C:294:GLU:OE2	1:C:294:GLU:O	2.30	0.49
1:D:5:LYS:HZ1	2:F:23:ARG:HD3	1.67	0.49
1:B:262:GLU:C	1:B:264:ASN:H	2.14	0.49
4:A:540:HOH:O	2:E:8:VAL:HB	2.13	0.48
1:A:190:HIS:HD2	4:A:446:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HB	1:B:142:LYS:HD2	1.94	0.48
1:B:249:SER:HB3	4:B:764:HOH:O	2.12	0.48
2:E:23:ARG:HA	4:E:419:HOH:O	2.13	0.48
1:D:294:GLU:OE2	1:D:317:ASP:OD1	2.32	0.48
1:B:162:ASN:HD22	1:B:261:GLY:HA2	1.79	0.48
1:C:248:ALA:HA	1:C:251:PHE:CZ	2.48	0.48
1:D:202:ASN:HD22	1:D:203:THR:H	1.62	0.48
1:D:252:TYR:HB2	1:D:257:TYR:CD1	2.48	0.47
1:D:215:LEU:HD13	1:D:221:ALA:HA	1.95	0.47
1:D:326:LEU:HG	1:D:338:ILE:HD12	1.95	0.47
1:A:3:ILE:HA	1:A:26:LEU:HD12	1.96	0.47
1:D:152:ILE:HG12	1:D:192:LEU:CD2	2.44	0.47
1:C:91:LYS:HZ2	1:C:91:LYS:HG3	1.34	0.47
1:D:259:LEU:HD22	1:D:267:PHE:CE1	2.49	0.47
1:D:7:ILE:N	1:D:7:ILE:CD1	2.77	0.47
1:D:300:PHE:HB3	1:D:334:ILE:HG23	1.96	0.47
1:C:31:VAL:CG1	2:F:6:LEU:HD12	2.42	0.47
1:B:300:PHE:HB3	1:B:334:ILE:HG23	1.96	0.47
1:B:145:MET:HG2	1:B:419:ALA:O	2.15	0.47
1:D:152:ILE:CB	4:D:737:HOH:O	2.61	0.47
1:B:300:PHE:CE2	1:B:318:LEU:HD13	2.50	0.47
1:D:9:ARG:HG3	1:D:11:ILE:HG23	1.97	0.46
1:B:424:ARG:HD2	4:B:744:HOH:O	2.14	0.46
1:D:41:SER:O	4:D:557:HOH:O	2.20	0.46
1:B:151:ASN:ND2	1:B:210:GLY:HA3	2.30	0.46
1:B:202:ASN:HD21	1:B:204:ALA:CB	2.29	0.46
1:D:152:ILE:CG2	1:D:153:ILE:N	2.78	0.46
1:C:237:GLY:O	1:C:424:ARG:NH2	2.49	0.46
1:B:150:MET:HE1	1:B:185:GLY:HA3	1.98	0.46
1:A:167:GLU:HG2	1:A:245:ASP:HB3	1.97	0.46
1:D:152:ILE:HG21	1:D:225:ILE:HG12	1.98	0.46
1:B:172:PRO:HG2	1:B:181:ALA:HB1	1.98	0.46
1:D:259:LEU:HD22	1:D:267:PHE:CD1	2.51	0.45
1:C:84:LYS:HE2	1:C:125:LYS:HG3	1.98	0.45
1:A:151:ASN:HD22	1:A:210:GLY:HA3	1.81	0.45
1:B:4:VAL:HG11	2:E:27:VAL:HG11	1.99	0.45
1:A:300:PHE:HB3	1:A:334:ILE:HG23	1.98	0.45
1:B:345:ILE:HG12	1:B:350:GLU:HB3	1.98	0.45
1:D:5:LYS:HZ2	2:F:23:ARG:NE	2.13	0.45
1:D:152:ILE:HG22	1:D:168:PHE:O	2.16	0.45
1:D:5:LYS:NZ	2:F:23:ARG:HD3	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ASN:HD22	1:D:203:THR:N	2.15	0.45
1:A:259:LEU:HD11	1:A:272:PHE:HE1	1.81	0.45
1:C:268:THR:O	1:C:271:GLU:N	2.49	0.45
1:A:245:ASP:HA	1:A:289:GLU:HB3	1.98	0.45
1:C:310:LYS:HB2	4:C:1265:HOH:O	2.16	0.45
1:C:256:LYS:HB3	1:C:256:LYS:HE3	1.53	0.45
1:A:237:GLY:O	1:A:424:ARG:NH1	2.46	0.45
1:B:202:ASN:HD22	1:B:204:ALA:H	1.63	0.44
1:A:84:LYS:HE2	1:A:125:LYS:CG	2.47	0.44
1:C:259:LEU:O	1:C:260:ALA:C	2.55	0.44
1:A:84:LYS:HE2	1:A:125:LYS:HG3	1.98	0.44
1:C:291:GLY:O	1:C:292:LEU:HD13	2.17	0.44
1:D:152:ILE:CG1	4:D:737:HOH:O	2.47	0.44
1:A:345:ILE:CG1	1:A:350:GLU:HB3	2.48	0.44
1:A:430:GLN:C	4:A:1166:HOH:O	2.56	0.44
1:C:292:LEU:HD13	1:C:303:GLN:HE22	1.83	0.44
1:B:260:ALA:C	1:B:262:GLU:N	2.71	0.44
1:C:252:TYR:HD1	1:C:257:TYR:CE1	2.31	0.44
1:A:101:ASN:H	1:A:101:ASN:HD22	1.64	0.44
1:D:327:LYS:N	1:D:357:MET:CE	2.81	0.43
1:B:262:GLU:C	1:B:264:ASN:N	2.72	0.43
1:B:197:LYS:HE3	1:B:197:LYS:HB3	1.73	0.43
1:B:268:THR:O	1:B:269:SER:C	2.53	0.43
1:B:5:LYS:HZ3	2:E:23:ARG:HG3	1.76	0.43
1:D:259:LEU:CD2	1:D:267:PHE:CE1	3.02	0.43
1:D:2:LYS:HG2	4:D:1029:HOH:O	2.18	0.43
1:C:323:THR:HA	1:C:357:MET:HE2	2.00	0.43
1:C:268:THR:O	1:C:269:SER:C	2.57	0.43
1:A:164:ASP:OD2	1:A:259:LEU:HB3	2.19	0.43
1:D:151:ASN:O	1:D:395:SER:HB2	2.19	0.43
1:C:1:SER:OG	1:C:84:LYS:HE3	2.18	0.43
2:E:24:TYR:HA	2:E:25:PRO:C	2.39	0.43
2:F:19:LYS:HE3	4:F:106:HOH:O	2.18	0.43
1:C:253:LYS:O	1:C:254:ASP:C	2.57	0.43
1:C:258:VAL:CA	1:C:259:LEU:HD23	2.49	0.43
1:C:92:ILE:O	1:C:96:LEU:HB2	2.18	0.43
1:A:249:SER:HB2	1:A:293:ASP:OD1	2.18	0.43
1:C:259:LEU:HD11	1:C:272:PHE:CE1	2.49	0.42
1:C:292:LEU:HD13	1:C:303:GLN:NE2	2.34	0.42
1:C:297:TRP:N	1:C:297:TRP:CD1	2.85	0.42
1:C:57:ARG:NH2	1:C:64:THR:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LYS:HE2	1:C:125:LYS:CG	2.50	0.42
4:C:436:HOH:O	1:D:402:VAL:CG2	2.64	0.42
1:D:398:ARG:HD2	1:D:398:ARG:HH11	1.67	0.42
1:D:171:GLN:HE22	1:D:286:VAL:CG2	2.33	0.42
1:D:145:MET:HG2	1:D:419:ALA:O	2.19	0.42
1:C:101:ASN:ND2	1:C:101:ASN:H	2.17	0.42
1:B:26:LEU:HD11	1:B:83:ALA:HB2	2.01	0.42
1:A:422:ASN:O	1:A:425:LYS:HD2	2.20	0.42
1:B:274:HIS:HA	1:B:277:GLU:HB2	2.02	0.42
2:E:4:MET:HG2	2:E:4:MET:O	2.20	0.42
1:D:245:ASP:HA	1:D:289:GLU:HB3	2.02	0.42
1:B:294:GLU:HG3	1:B:294:GLU:H	1.50	0.41
1:B:272:PHE:O	1:B:275:PHE:HB3	2.21	0.41
1:D:152:ILE:HG23	1:D:153:ILE:N	2.35	0.41
1:A:215:LEU:HD13	1:A:221:ALA:HA	2.02	0.41
1:B:304:THR:O	1:B:308:GLY:HA3	2.20	0.41
1:A:375:GLU:O	2:E:19:LYS:NZ	2.46	0.41
1:D:252:TYR:CD1	1:D:257:TYR:CD1	3.05	0.41
1:C:263:GLY:O	1:C:264:ASN:C	2.57	0.41
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.90	0.41
1:B:264:ASN:O	1:B:265:LYS:C	2.57	0.41
1:C:9:ARG:HG3	1:C:11:ILE:HG23	2.02	0.41
1:A:96:LEU:HD13	1:A:105:PHE:CZ	2.56	0.41
1:D:40:ALA:H	1:D:371:SER:HB2	1.85	0.41
1:B:294:GLU:HG3	4:B:764:HOH:O	2.20	0.41
1:A:199:LYS:HB3	1:A:199:LYS:HE3	1.94	0.41
1:A:290:ASP:OD2	1:A:316:ASP:HB3	2.21	0.41
4:A:435:HOH:O	1:B:402:VAL:HG23	2.19	0.40
1:D:410:ARG:HB3	2:F:10:ALA:HB2	2.02	0.40
1:B:145:MET:HE2	1:B:178:VAL:HG11	2.03	0.40
1:A:313:LEU:O	1:A:335:ALA:HB1	2.20	0.40
1:B:316:ASP:HB2	1:B:339:LEU:HD22	2.02	0.40
1:C:384:VAL:HG11	1:C:411:ILE:HG21	2.03	0.40
1:B:213:PRO:HG2	1:B:215:LEU:HG	2.04	0.40
1:B:91:LYS:NZ	1:B:95:ASP:OD2	2.41	0.40
1:D:46:GLU:CD	1:D:344:GLN:HG2	2.42	0.40
1:C:215:LEU:HD13	1:C:221:ALA:HA	2.04	0.40
1:B:10:GLU:HG3	1:B:63:VAL:HG22	2.03	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	429/432 (99%)	415 (97%)	12 (3%)	2 (0%)	34	21
1	B	428/432 (99%)	415 (97%)	10 (2%)	3 (1%)	26	14
1	C	428/432 (99%)	407 (95%)	18 (4%)	3 (1%)	26	14
1	D	429/432 (99%)	417 (97%)	11 (3%)	1 (0%)	52	42
2	E	26/28 (93%)	26 (100%)	0	0	100	100
2	F	23/28 (82%)	23 (100%)	0	0	100	100
All	All	1763/1784 (99%)	1703 (97%)	51 (3%)	9 (0%)	34	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	ASN
1	B	261	GLY
1	B	398	ARG
1	C	248	ALA
1	A	335	ALA
1	A	398	ARG
1	B	335	ALA
1	C	398	ARG
1	D	398	ARG

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	324/326 (99%)	311 (96%)	13 (4%)	38 26
1	B	321/326 (98%)	297 (92%)	24 (8%)	17 7
1	C	324/326 (99%)	296 (91%)	28 (9%)	13 5
1	D	317/326 (97%)	303 (96%)	14 (4%)	35 22
2	E	23/23 (100%)	22 (96%)	1 (4%)	35 23
2	F	20/23 (87%)	19 (95%)	1 (5%)	30 18
All	All	1329/1350 (98%)	1248 (94%)	81 (6%)	23 11

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	76	GLN
1	A	96	LEU
1	A	101	ASN
1	A	142	LYS
1	A	238	LYS
1	A	253	LYS
1	A	265	LYS
1	A	307	LEU
1	A	342	PHE
1	A	369	HIS
1	A	400	ASP
1	A	425	LYS
1	B	26	LEU
1	B	38	SER
1	B	48	LEU
1	B	101	ASN
1	B	111	LEU
1	B	152	ILE
1	B	157	GLU
1	B	162	ASN
1	B	202	ASN
1	B	214	ASN
1	B	253	LYS
1	B	273	THR
1	B	277	GLU
1	B	294	GLU
1	B	311	ILE
1	B	317	ASP
1	B	326	LEU

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Mol	Chain	Res	Type
1	B	327	LYS
1	B	342	PHE
1	B	359	LYS
1	B	369	HIS
1	B	400	ASP
1	B	424	ARG
1	B	425	LYS
1	C	26	LEU
1	C	41	SER
1	C	42	THR
1	C	48	LEU
1	C	56	SER
1	C	57	ARG
1	C	91	LYS
1	C	96	LEU
1	C	101	ASN
1	C	157	GLU
1	C	176	LYS
1	C	238	LYS
1	C	254	ASP
1	C	256	LYS
1	C	259	LEU
1	C	264	ASN
1	C	278	GLU
1	C	292	LEU
1	C	294	GLU
1	C	306	VAL
1	C	307	LEU
1	C	309	ASP
1	C	318	LEU
1	C	342	PHE
1	C	369	HIS
1	C	400	ASP
1	C	418	LYS
1	C	428	LYS
1	D	5	LYS
1	D	7	ILE
1	D	48	LEU
1	D	101	ASN
1	D	111	LEU
1	D	154	ASN
1	D	202	ASN

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Mol	Chain	Res	Type
1	D	236	LEU
1	D	259	LEU
1	D	326	LEU
1	D	342	PHE
1	D	343	ASN
1	D	369	HIS
1	D	400	ASP
2	E	8	VAL
2	F	1	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	137	ASN
1	A	151	ASN
1	A	154	ASN
1	A	171	GLN
1	A	190	HIS
1	A	430	GLN
1	B	76	GLN
1	B	101	ASN
1	B	137	ASN
1	B	151	ASN
1	B	154	ASN
1	B	162	ASN
1	B	171	GLN
1	B	190	HIS
1	B	191	HIS
1	B	202	ASN
1	B	264	ASN
1	C	25	HIS
1	C	76	GLN
1	C	101	ASN
1	C	158	HIS
1	C	166	GLN
1	C	171	GLN
1	C	190	HIS
1	C	202	ASN
1	C	274	HIS
1	C	282	GLN
1	C	303	GLN

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Mol	Chain	Res	Type
1	C	430	GLN
1	D	76	GLN
1	D	101	ASN
1	D	137	ASN
1	D	171	GLN
1	D	190	HIS
1	D	191	HIS
1	D	202	ASN
1	D	274	HIS

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	430/432 (99%)	-0.07	4 (0%) 85 87	8, 16, 29, 37	0
1	B	430/432 (99%)	0.34	28 (6%) 22 25	10, 22, 50, 68	0
1	C	430/432 (99%)	0.49	51 (11%) 6 6	11, 23, 57, 69	0
1	D	431/432 (99%)	0.21	21 (4%) 33 36	10, 21, 39, 54	0
2	E	28/28 (100%)	0.68	4 (14%) 4 4	14, 21, 31, 36	0
2	F	25/28 (89%)	1.99	9 (36%) 0 0	20, 26, 31, 41	0
All	All	1774/1784 (99%)	0.27	117 (6%) 22 24	8, 20, 47, 69	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	25	PRO	9.3
1	D	431	ALA	7.0
1	C	253	LYS	6.3
1	C	263	GLY	6.3
1	D	162	ASN	6.1
1	C	254	ASP	5.9
1	D	257	TYR	5.6
1	B	263	GLY	5.5
1	B	264	ASN	5.5
1	C	44	SER	5.5
1	B	254	ASP	5.1
2	F	23	ARG	5.0
1	B	253	LYS	4.7
1	C	302	TYR	4.7
1	C	266	ALA	4.7
2	E	1	GLN	4.4
1	D	160	ASP	4.4
1	D	157	GLU	4.4
1	C	42	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	258	VAL	4.3
1	C	40	ALA	4.3
2	F	24	TYR	4.1
1	C	255	GLY	4.0
1	B	261	GLY	4.0
1	C	281	LYS	3.8
1	C	160	ASP	3.8
1	C	305	LYS	3.8
1	B	216	GLY	3.7
1	C	331	GLU	3.6
1	C	258	VAL	3.6
1	C	256	LYS	3.6
1	B	265	LYS	3.5
1	C	252	TYR	3.5
1	D	42	THR	3.4
1	C	257	TYR	3.4
1	C	298	ASP	3.3
1	B	162	ASN	3.3
1	D	317	ASP	3.2
2	F	1	GLN	3.2
1	D	158	HIS	3.2
1	B	302	TYR	3.2
1	C	43	GLY	3.2
1	B	42	THR	3.1
1	C	100	GLU	3.1
2	F	5	PRO	3.1
1	D	305	LYS	3.1
1	B	260	ALA	3.1
1	C	282	GLN	3.0
1	C	278	GLU	3.0
1	C	317	ASP	3.0
1	A	100	GLU	3.0
1	B	266	ALA	3.0
1	B	288	ILE	3.0
1	C	262	GLU	3.0
1	D	254	ASP	2.9
1	B	309	ASP	2.8
1	C	274	HIS	2.8
1	D	56	SER	2.8
1	C	306	VAL	2.7
1	B	256	LYS	2.7
1	C	162	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	271	GLU	2.7
1	B	305	LYS	2.7
1	D	45	ARG	2.7
1	D	41	SER	2.6
1	B	200	GLY	2.6
1	C	142	LYS	2.6
1	D	265	LYS	2.6
1	D	48	LEU	2.6
1	B	219	ALA	2.6
1	C	276	LEU	2.6
1	C	328	GLU	2.6
1	B	276	LEU	2.6
1	C	115	LEU	2.6
1	C	243	ALA	2.6
1	B	243	ALA	2.5
1	D	314	VAL	2.5
1	C	214	ASN	2.5
1	B	331	GLU	2.5
2	F	7	THR	2.5
2	F	8	VAL	2.5
1	A	254	ASP	2.5
1	C	309	ASP	2.5
1	C	275	PHE	2.4
1	A	314	VAL	2.4
1	C	300	PHE	2.4
1	C	327	LYS	2.4
1	C	283	TYR	2.3
1	B	238	LYS	2.3
1	B	262	GLU	2.3
1	D	309	ASP	2.3
1	D	252	TYR	2.3
1	C	310	LYS	2.3
1	B	273	THR	2.3
1	C	39	GLY	2.3
1	B	282	GLN	2.3
1	C	318	LEU	2.2
1	C	314	VAL	2.2
1	C	268	THR	2.2
1	C	157	GLU	2.2
1	C	270	GLU	2.2
1	C	244	MET	2.2
1	D	274	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	265	LYS	2.2
1	D	159	ALA	2.1
2	F	22	ILE	2.1
2	F	15	LEU	2.1
1	A	309	ASP	2.1
2	E	8	VAL	2.1
1	C	272	PHE	2.1
2	E	28	ARG	2.1
1	C	237	GLY	2.1
1	C	299	GLY	2.1
1	B	259	LEU	2.0
1	B	55	LYS	2.0
1	B	297	TRP	2.0
2	E	16	ALA	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	MG	A	1431	1/1	0.98	0.05	-2.00	25,25,25,25	0
3	MG	C	1431	1/1	0.96	0.05	-3.28	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.