



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 1T5O / pdb_00001t5o
Title : Crystal structure of the translation initiation factor eIF-2B, subunit delta, from *A. fulgidus*
Authors : Malashkevich, V.N.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-05-04
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

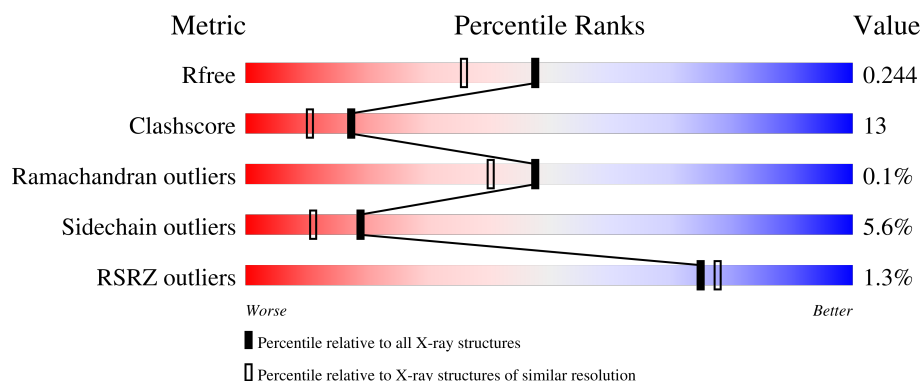
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	2% 68% 24% • • •
1	B	351	% 76% 19% • •
1	C	351	% 74% 20% • •
1	D	351	% 67% 26% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12002 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 Translation initiation factor eIF2B, subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	B	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	C	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	D	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP O29877
A	2	SER	-	cloning artifact	UNP O29877
A	3	LEU	-	cloning artifact	UNP O29877
A	342	GLU	-	cloning artifact	UNP O29877
A	343	GLY	-	cloning artifact	UNP O29877
A	344	GLY	-	cloning artifact	UNP O29877
A	345	SER	-	cloning artifact	UNP O29877
A	346	HIS	-	expression tag	UNP O29877
A	347	HIS	-	expression tag	UNP O29877
A	348	HIS	-	expression tag	UNP O29877
A	349	HIS	-	expression tag	UNP O29877
A	350	HIS	-	expression tag	UNP O29877
A	351	HIS	-	expression tag	UNP O29877
B	1	MET	-	cloning artifact	UNP O29877
B	2	SER	-	cloning artifact	UNP O29877
B	3	LEU	-	cloning artifact	UNP O29877
B	342	GLU	-	cloning artifact	UNP O29877
B	343	GLY	-	cloning artifact	UNP O29877
B	344	GLY	-	cloning artifact	UNP O29877
B	345	SER	-	cloning artifact	UNP O29877
B	346	HIS	-	expression tag	UNP O29877

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	HIS	-	expression tag	UNP O29877
B	348	HIS	-	expression tag	UNP O29877
B	349	HIS	-	expression tag	UNP O29877
B	350	HIS	-	expression tag	UNP O29877
B	351	HIS	-	expression tag	UNP O29877
C	1	MET	-	cloning artifact	UNP O29877
C	2	SER	-	cloning artifact	UNP O29877
C	3	LEU	-	cloning artifact	UNP O29877
C	342	GLU	-	cloning artifact	UNP O29877
C	343	GLY	-	cloning artifact	UNP O29877
C	344	GLY	-	cloning artifact	UNP O29877
C	345	SER	-	cloning artifact	UNP O29877
C	346	HIS	-	expression tag	UNP O29877
C	347	HIS	-	expression tag	UNP O29877
C	348	HIS	-	expression tag	UNP O29877
C	349	HIS	-	expression tag	UNP O29877
C	350	HIS	-	expression tag	UNP O29877
C	351	HIS	-	expression tag	UNP O29877
D	1	MET	-	cloning artifact	UNP O29877
D	2	SER	-	cloning artifact	UNP O29877
D	3	LEU	-	cloning artifact	UNP O29877
D	342	GLU	-	cloning artifact	UNP O29877
D	343	GLY	-	cloning artifact	UNP O29877
D	344	GLY	-	cloning artifact	UNP O29877
D	345	SER	-	cloning artifact	UNP O29877
D	346	HIS	-	expression tag	UNP O29877
D	347	HIS	-	expression tag	UNP O29877
D	348	HIS	-	expression tag	UNP O29877
D	349	HIS	-	expression tag	UNP O29877
D	350	HIS	-	expression tag	UNP O29877
D	351	HIS	-	expression tag	UNP O29877

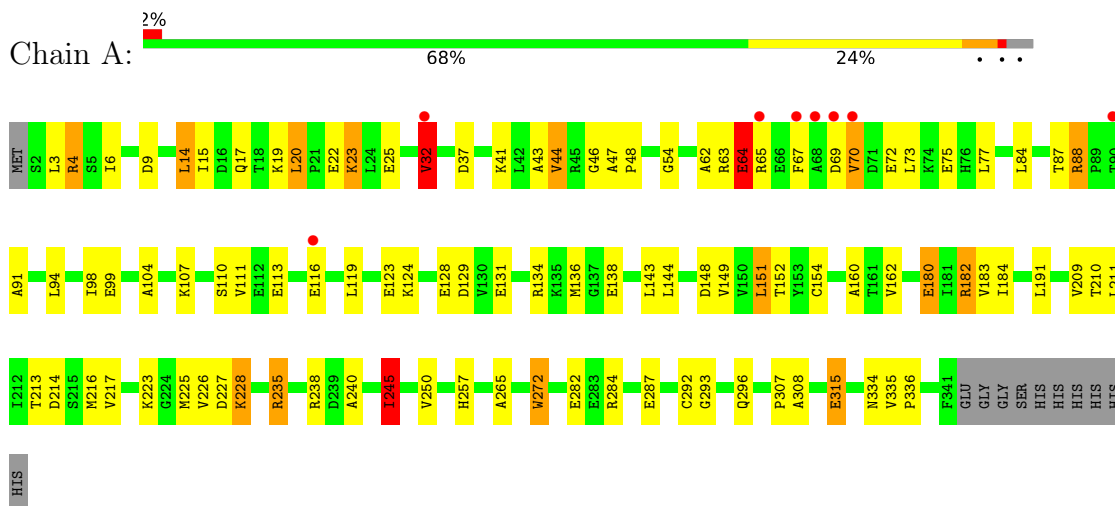
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	325	Total O 325 325	0	0
2	B	396	Total O 396 396	0	0
2	C	374	Total O 374 374	0	0
2	D	303	Total O 303 303	0	0

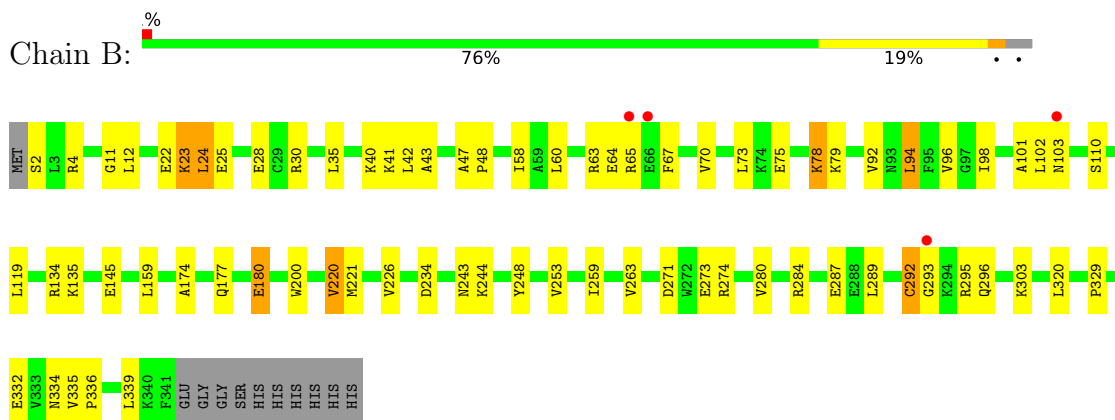
3 Residue-property plots [i](#)

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

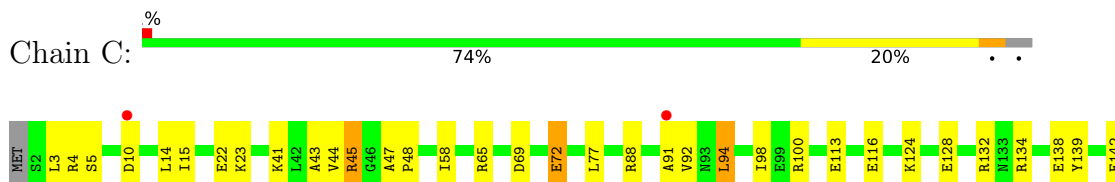
- Molecule 1: Translation initiation factor eIF2B, subunit delta

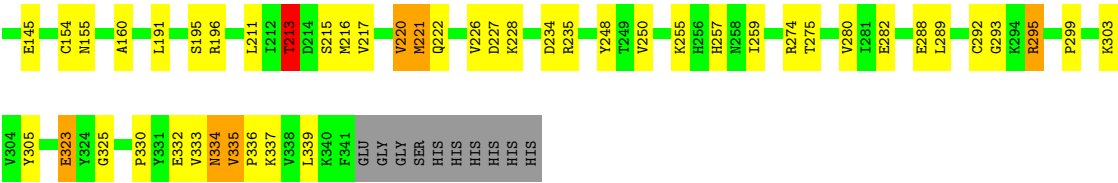


- Molecule 1: Translation initiation factor eIF2B, subunit delta



- Molecule 1: Translation initiation factor eIF2B, subunit delta





• Molecule 1: Translation initiation factor eIF2B, subunit delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.58Å 110.20Å 141.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 1.90 9.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (9.99-1.90) 92.9 (9.99-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.246 0.194 , 0.244	Depositor DCC
R_{free} test set	8765 reflections (7.20%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12002	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3830e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.65	1/2694 (0.0%)	1.04	14/3652 (0.4%)
1	B	0.69	0/2694	1.01	9/3652 (0.2%)
1	C	0.71	2/2694 (0.1%)	1.05	13/3652 (0.4%)
1	D	0.70	2/2694 (0.1%)	1.06	20/3652 (0.5%)
All	All	0.69	5/10776 (0.0%)	1.04	56/14608 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	MET	SD-CE	-9.14	1.56	1.79
1	C	335	VAL	CA-CB	6.18	1.57	1.54
1	C	221	MET	SD-CE	-5.68	1.65	1.79
1	D	203	MET	SD-CE	-5.68	1.65	1.79
1	A	136	MET	SD-CE	-5.22	1.66	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ARG	CA-C-N	8.76	130.79	119.84
1	C	88	ARG	C-N-CA	8.76	130.79	119.84
1	D	334	ASN	N-CA-C	8.23	121.37	111.82
1	C	4	ARG	N-CA-C	-7.98	99.99	110.53
1	A	293	GLY	N-CA-C	-7.75	94.82	113.18
1	A	4	ARG	N-CA-C	-7.40	100.56	110.55
1	A	334	ASN	N-CA-C	7.39	121.54	112.23
1	B	293	GLY	N-CA-C	-7.08	97.83	110.86
1	A	88	ARG	CA-C-N	6.99	127.58	119.47
1	A	88	ARG	C-N-CA	6.99	127.58	119.47
1	D	15	ILE	N-CA-C	-6.75	100.87	109.30
1	D	238	ARG	N-CA-C	6.57	119.27	111.71
1	D	4	ARG	N-CA-C	-6.48	101.97	110.53
1	C	43	ALA	N-CA-C	-6.43	104.36	111.82
1	C	94	LEU	N-CA-C	-6.41	104.22	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	10	ASP	N-CA-C	-6.17	104.11	112.26
1	C	293	GLY	N-CA-C	-6.17	100.45	110.95
1	D	43	ALA	N-CA-C	-6.15	104.69	111.82
1	D	32	VAL	N-CA-C	-6.09	105.08	113.00
1	D	240	ALA	N-CA-C	6.07	118.08	108.79
1	A	240	ALA	N-CA-C	6.07	117.76	108.42
1	A	15	ILE	N-CA-C	-6.04	100.91	108.89
1	A	70	VAL	N-CA-C	5.97	116.15	110.42
1	D	94	LEU	N-CA-C	-5.93	104.82	111.28
1	B	334	ASN	N-CA-C	5.92	119.69	112.23
1	D	245	ILE	CB-CA-C	-5.83	101.89	111.51
1	A	245	ILE	CB-CA-C	-5.69	102.13	111.51
1	D	88	ARG	CA-C-N	5.69	126.95	119.84
1	D	88	ARG	C-N-CA	5.69	126.95	119.84
1	D	329	PRO	N-CA-C	-5.64	105.05	110.47
1	A	272	TRP	N-CA-C	5.63	119.77	113.01
1	D	192	ASN	N-CA-C	5.61	119.31	111.74
1	B	4	ARG	N-CA-C	-5.59	103.15	110.53
1	A	43	ALA	N-CA-C	-5.58	105.35	111.82
1	D	305	TYR	N-CA-C	-5.54	99.39	108.41
1	D	279	VAL	N-CA-C	5.52	116.52	108.58
1	D	293	GLY	N-CA-C	-5.46	100.25	113.18
1	B	23	LYS	N-CA-C	5.45	117.13	108.79
1	B	329	PRO	N-CA-C	-5.42	104.09	110.70
1	A	238	ARG	N-CA-C	5.41	118.98	112.38
1	A	32	VAL	CB-CA-C	-5.39	104.98	111.88
1	C	334	ASN	N-CA-C	5.34	118.02	111.82
1	D	162	VAL	N-CA-C	-5.31	105.36	110.72
1	D	68	ALA	N-CA-C	-5.28	106.07	112.88
1	B	64	GLU	N-CA-C	5.28	117.71	111.33
1	C	274	ARG	N-CA-C	5.27	117.42	109.41
1	C	213	THR	N-CA-C	-5.26	103.44	110.55
1	B	63	ARG	CA-C-N	5.26	127.58	120.38
1	B	63	ARG	C-N-CA	5.26	127.58	120.38
1	C	196	ARG	N-CA-C	5.24	117.07	111.36
1	D	272	TRP	N-CA-C	5.21	118.73	112.38
1	D	271	ASP	N-CA-C	-5.19	100.01	109.56
1	C	154	CYS	CB-CA-C	-5.10	110.67	116.54
1	B	94	LEU	N-CA-C	-5.07	105.64	111.07
1	C	22	GLU	N-CA-C	5.03	116.77	111.28
1	A	154	CYS	CB-CA-C	-5.01	110.81	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2651	0	2696	90	0
1	B	2651	0	2696	56	0
1	C	2651	0	2696	58	0
1	D	2651	0	2696	87	0
2	A	325	0	0	19	0
2	B	396	0	0	14	0
2	C	374	0	0	10	0
2	D	303	0	0	13	0
All	All	12002	0	10784	266	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 13.

All (266) 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:132:ARG:HG3	1:C:323:GLU:HG2	1.32	1.07
1:D:6:ILE:HD12	1:D:14:LEU:HD21	1.44	0.96
1:C:235:ARG:HG2	2:C:699:HOH:O	1.69	0.92
1:D:22:GLU:HG2	2:D:463:HOH:O	1.70	0.91
1:A:22:GLU:HG2	1:A:23:LYS:HG3	1.55	0.88
1:C:132:ARG:CG	1:C:323:GLU:HG2	2.02	0.88
1:D:136:MET:CE	1:D:166:THR:HA	2.05	0.86
1:C:299:PRO:HG2	1:D:203:MET:CE	2.07	0.85
1:A:182:ARG:HH11	1:A:182:ARG:HB2	1.41	0.84
1:D:315:GLU:HG3	2:D:585:HOH:O	1.77	0.84
1:C:134:ARG:O	1:C:138:GLU:HG2	1.75	0.84
1:D:245:ILE:HG12	1:D:307:PRO:O	1.77	0.83
1:B:58:ILE:HD12	1:B:101:ALA:HB3	1.61	0.81
1:A:65:ARG:HB2	2:A:519:HOH:O	1.80	0.81
1:A:245:ILE:HG12	1:A:307:PRO:O	1.81	0.80
1:B:23:LYS:HD3	1:B:25:GLU:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD22	1:D:44:VAL:HG12	1.64	0.80
1:A:149:VAL:HG11	1:A:225:MET:O	1.80	0.79
1:A:296:GLN:OE1	1:B:22:GLU:HG2	1.82	0.79
1:D:22:GLU:HB3	2:D:442:HOH:O	1.83	0.79
1:D:146:ASP:OD1	1:D:180:GLU:HG3	1.82	0.78
1:D:136:MET:HE1	1:D:166:THR:HA	1.65	0.78
1:C:299:PRO:HG2	1:D:203:MET:HE1	1.66	0.77
1:D:69:ASP:HB3	1:D:72:GLU:HB2	1.67	0.77
1:A:149:VAL:HG12	1:A:227:ASP:OD2	1.86	0.76
1:C:282:GLU:CD	1:C:282:GLU:H	1.93	0.76
1:B:273:GLU:HG2	2:B:612:HOH:O	1.84	0.75
1:A:143:LEU:O	1:A:228:LYS:HE3	1.88	0.74
1:B:70:VAL:HG23	2:B:402:HOH:O	1.87	0.73
1:A:214:ASP:O	1:A:217:VAL:HG23	1.89	0.72
1:B:23:LYS:HD2	1:B:25:GLU:OE2	1.89	0.72
1:A:75:GLU:HG3	2:A:528:HOH:O	1.90	0.71
1:C:292:CYS:CB	1:D:292:CYS:HG	2.04	0.70
1:D:99:GLU:HG3	2:D:446:HOH:O	1.90	0.70
1:A:113:GLU:HG2	2:A:488:HOH:O	1.90	0.70
1:C:195:SER:HB3	1:D:297:ILE:O	1.92	0.69
1:C:299:PRO:CG	1:D:203:MET:HE1	2.21	0.69
1:A:32:VAL:HG13	2:A:552:HOH:O	1.92	0.69
1:A:128:GLU:HA	1:A:131:GLU:HG2	1.72	0.69
1:A:287:GLU:HG3	2:A:648:HOH:O	1.93	0.69
1:D:6:ILE:CD1	1:D:14:LEU:HD21	2.23	0.69
1:A:47:ALA:HB3	1:A:48:PRO:HD3	1.76	0.68
1:A:138:GLU:HG3	2:A:440:HOH:O	1.94	0.68
1:A:69:ASP:OD1	1:A:72:GLU:HG3	1.94	0.68
1:C:299:PRO:HG2	1:D:203:MET:HE3	1.75	0.68
1:D:36:ALA:O	1:D:40:LYS:HG3	1.94	0.68
1:B:65:ARG:HD3	2:B:725:HOH:O	1.95	0.67
1:A:6:ILE:HG13	1:A:14:LEU:HD23	1.77	0.67
1:D:200:TRP:CZ2	1:D:204:GLU:HG3	2.29	0.67
1:A:265:ALA:HB3	2:A:531:HOH:O	1.94	0.66
1:C:292:CYS:HG	1:D:292:CYS:CB	2.09	0.66
1:C:23:LYS:HE2	2:C:499:HOH:O	1.96	0.65
1:C:221:MET:SD	1:C:259:ILE:HD12	2.38	0.64
1:D:47:ALA:HB3	1:D:48:PRO:HD3	1.79	0.64
1:D:14:LEU:HD22	1:D:44:VAL:CG1	2.26	0.64
1:D:136:MET:HE1	1:D:166:THR:CB	2.28	0.64
1:A:14:LEU:HD13	1:A:44:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HD22	1:C:44:VAL:HG21	1.79	0.63
1:B:22:GLU:HG3	2:B:404:HOH:O	1.99	0.63
1:A:182:ARG:HH11	1:A:182:ARG:CB	2.12	0.63
1:D:23:LYS:HE2	1:D:25:GLU:HG2	1.81	0.62
1:D:78:LYS:O	1:D:78:LYS:HD3	1.98	0.62
1:C:334:ASN:HA	1:C:337:LYS:HG2	1.81	0.62
1:D:78:LYS:HD3	1:D:78:LYS:C	2.24	0.62
1:D:124:LYS:O	1:D:128:GLU:HG3	2.01	0.61
1:A:180:GLU:HG3	1:A:180:GLU:O	1.99	0.61
1:D:136:MET:HE1	1:D:166:THR:CA	2.31	0.60
1:C:14:LEU:HD22	1:C:44:VAL:CG2	2.31	0.60
1:C:124:LYS:O	1:C:128:GLU:HG3	2.01	0.60
1:A:151:LEU:HD12	1:A:152:THR:N	2.16	0.60
1:B:135:LYS:HD2	2:B:675:HOH:O	2.02	0.60
1:B:11:GLY:HA3	1:B:30:ARG:NH2	2.17	0.59
1:D:136:MET:HE1	1:D:166:THR:HG22	1.85	0.59
1:B:47:ALA:HB3	1:B:48:PRO:HD3	1.85	0.59
1:B:332:GLU:OE1	1:B:332:GLU:N	2.29	0.58
1:A:41:LYS:HD3	2:A:529:HOH:O	2.03	0.58
1:B:11:GLY:HA3	1:B:30:ARG:HH22	1.69	0.58
1:A:128:GLU:HA	1:A:131:GLU:CG	2.33	0.58
1:A:94:LEU:O	1:A:98:ILE:HG12	2.04	0.58
1:C:280:VAL:HG23	1:C:280:VAL:O	2.03	0.58
1:C:303:LYS:HD2	2:D:629:HOH:O	2.03	0.57
1:D:58:ILE:HD12	1:D:101:ALA:HB3	1.86	0.57
2:A:493:HOH:O	1:B:303:LYS:HD3	2.04	0.57
1:D:182:ARG:NH2	2:D:481:HOH:O	2.37	0.56
1:A:227:ASP:C	1:A:228:LYS:HG2	2.31	0.56
1:D:61:ALA:HA	1:D:64:GLU:HG3	1.88	0.56
1:C:65:ARG:NH2	2:C:669:HOH:O	2.38	0.56
1:C:333:VAL:HG12	1:C:337:LYS:HE3	1.88	0.56
1:D:273:GLU:HG3	2:D:352:HOH:O	2.05	0.56
1:A:37:ASP:O	1:A:41:LYS:HG3	2.06	0.55
1:B:134:ARG:NH1	2:B:441:HOH:O	2.39	0.55
1:C:332:GLU:HG2	2:C:385:HOH:O	2.06	0.55
1:D:30:ARG:N	1:D:34:GLU:OE2	2.39	0.55
1:C:132:ARG:NH1	2:C:462:HOH:O	2.38	0.55
1:C:91:ALA:O	1:C:92:VAL:HB	2.06	0.55
1:A:213:THR:HG22	1:A:216:MET:CG	2.37	0.54
1:D:109:GLU:OE2	1:D:109:GLU:HA	2.06	0.54
1:C:255:LYS:NZ	2:C:458:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:VAL:HG11	1:C:250:VAL:HG22	1.90	0.53
1:C:128:GLU:HB3	2:C:462:HOH:O	2.07	0.53
1:D:22:GLU:HG3	1:D:23:LYS:N	2.23	0.53
1:C:47:ALA:HB3	1:C:48:PRO:HD3	1.90	0.53
1:A:70:VAL:HG21	1:A:110:SER:HA	1.90	0.53
1:A:213:THR:HG22	1:A:216:MET:HG3	1.89	0.53
1:A:84:LEU:O	1:A:87:THR:HG23	2.08	0.53
1:D:26:VAL:HB	2:D:574:HOH:O	2.08	0.53
1:A:62:ALA:HB2	1:A:77:LEU:HD21	1.90	0.52
1:A:23:LYS:HE3	2:A:549:HOH:O	2.09	0.52
1:A:88:ARG:HG3	1:A:91:ALA:HB2	1.90	0.52
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.72	0.52
1:B:180:GLU:HG2	2:B:428:HOH:O	2.09	0.52
1:D:110:SER:OG	1:D:113:GLU:HB2	2.09	0.52
1:B:220:VAL:HG13	1:B:226:VAL:HG23	1.92	0.52
1:C:58:ILE:HD11	1:C:98:ILE:HG23	1.91	0.52
1:A:23:LYS:HZ2	1:A:25:GLU:HG3	1.74	0.51
1:A:63:ARG:O	1:A:64:GLU:C	2.51	0.51
1:A:124:LYS:O	1:A:128:GLU:HG3	2.10	0.51
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.92	0.51
1:D:60:LEU:O	1:D:64:GLU:HG3	2.10	0.51
1:B:103:ASN:HB2	2:B:388:HOH:O	2.11	0.51
1:C:292:CYS:SG	1:D:292:CYS:CB	2.99	0.51
1:A:151:LEU:HD12	1:A:152:THR:H	1.75	0.50
1:D:14:LEU:HD13	1:D:44:VAL:CG1	2.41	0.50
1:B:58:ILE:CD1	1:B:98:ILE:O	2.59	0.50
1:C:100:ARG:HG2	1:C:100:ARG:HH11	1.77	0.50
1:A:70:VAL:HG23	2:A:563:HOH:O	2.11	0.50
1:A:128:GLU:HA	1:A:131:GLU:CD	2.36	0.50
1:D:16:ASP:HB2	1:D:27:ILE:HG13	1.93	0.49
1:A:235:ARG:CZ	2:A:624:HOH:O	2.60	0.49
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.95	0.49
1:B:22:GLU:HB3	2:B:634:HOH:O	2.13	0.49
1:B:271:ASP:OD2	1:B:274:ARG:HD2	2.12	0.49
1:A:119:LEU:O	1:A:123:GLU:HG3	2.13	0.49
1:B:28:GLU:CD	1:B:30:ARG:HH21	2.21	0.49
1:B:40:LYS:HE2	2:B:521:HOH:O	2.11	0.49
1:D:31:ASN:C	1:D:33:GLU:H	2.19	0.49
1:B:40:LYS:CE	2:B:521:HOH:O	2.59	0.49
1:D:107:LYS:HB2	1:D:107:LYS:NZ	2.27	0.49
1:A:88:ARG:HG3	1:A:88:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:CA	1:A:131:GLU:HG2	2.40	0.49
1:A:32:VAL:HG22	2:A:552:HOH:O	2.12	0.49
1:C:213:THR:CG2	1:C:215:SER:OG	2.61	0.48
1:A:213:THR:HG22	1:A:216:MET:SD	2.53	0.48
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.95	0.48
1:C:227:ASP:C	1:C:228:LYS:HG2	2.38	0.48
1:D:284:ARG:HD2	2:D:385:HOH:O	2.13	0.48
1:D:136:MET:HE1	1:D:166:THR:CG2	2.42	0.48
1:D:199:CYS:HB3	1:D:203:MET:HE2	1.95	0.48
1:A:107:LYS:HE3	2:A:601:HOH:O	2.13	0.48
1:C:295:ARG:HD2	1:D:293:GLY:HA2	1.95	0.48
1:A:17:GLN:HA	1:A:20:LEU:HD22	1.96	0.48
1:B:40:LYS:NZ	2:B:521:HOH:O	2.38	0.48
1:D:99:GLU:HG3	2:D:434:HOH:O	2.13	0.48
1:A:22:GLU:HB3	2:A:484:HOH:O	2.12	0.48
1:C:45:ARG:NH2	1:C:155:ASN:OD1	2.46	0.48
1:D:58:ILE:CD1	1:D:98:ILE:O	2.62	0.48
1:C:292:CYS:CB	1:D:292:CYS:SG	3.00	0.47
1:D:183:VAL:O	1:D:209:VAL:HA	2.14	0.47
1:A:151:LEU:CD1	1:A:184:ILE:O	2.62	0.47
1:D:75:GLU:HG3	2:D:650:HOH:O	2.13	0.47
1:A:148:ASP:OD1	1:A:228:LYS:HE2	2.15	0.47
1:A:182:ARG:HH11	1:A:182:ARG:CG	2.28	0.47
1:A:128:GLU:O	1:A:131:GLU:HG2	2.15	0.47
1:A:272:TRP:HB3	2:A:556:HOH:O	2.14	0.47
1:C:213:THR:HB	1:C:216:MET:HE3	1.97	0.47
1:A:151:LEU:HD12	1:A:184:ILE:O	2.15	0.46
1:D:31:ASN:C	1:D:33:GLU:N	2.70	0.46
1:B:28:GLU:CD	1:B:30:ARG:HE	2.23	0.46
1:B:280:VAL:O	1:B:280:VAL:HG23	2.14	0.46
1:B:295:ARG:HD2	1:B:295:ARG:HA	1.76	0.46
1:C:69:ASP:HB3	1:C:72:GLU:HB2	1.96	0.46
1:A:104:ALA:O	1:A:107:LYS:HB2	2.15	0.46
1:C:5:SER:HA	1:C:15:ILE:HD12	1.98	0.46
1:C:45:ARG:NH2	1:C:160:ALA:HB2	2.31	0.46
1:B:58:ILE:HD11	1:B:98:ILE:O	2.16	0.46
1:D:6:ILE:HB	1:D:14:LEU:HD23	1.98	0.46
1:D:62:ALA:HA	1:D:73:LEU:HD11	1.98	0.46
1:D:94:LEU:HD23	1:D:94:LEU:C	2.41	0.46
1:A:70:VAL:HG22	1:A:111:VAL:N	2.31	0.46
1:C:289:LEU:HD11	1:D:213:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLU:OE1	1:D:258:ASN:ND2	2.49	0.45
1:B:2:SER:HB3	2:B:636:HOH:O	2.15	0.45
1:C:303:LYS:HD3	1:D:210:THR:OG1	2.17	0.45
1:B:24:LEU:HG	1:B:200:TRP:CZ2	2.51	0.45
1:D:67:PHE:CE2	1:D:73:LEU:HA	2.51	0.45
1:A:88:ARG:HG3	1:A:91:ALA:CB	2.45	0.45
1:A:46:GLY:HA3	1:A:160:ALA:O	2.16	0.45
1:A:149:VAL:HG13	1:A:227:ASP:H	1.81	0.45
1:C:222:GLN:HG3	1:D:248:TYR:CE1	2.51	0.45
1:A:149:VAL:HG13	1:A:226:VAL:HA	1.97	0.45
1:B:30:ARG:NH2	2:B:412:HOH:O	2.48	0.45
1:B:78:LYS:HD3	1:B:78:LYS:O	2.16	0.45
1:D:6:ILE:CB	1:D:14:LEU:HD23	2.47	0.45
1:C:289:LEU:HD11	1:D:213:THR:HG22	1.99	0.45
1:A:23:LYS:NZ	1:A:25:GLU:HG3	2.32	0.45
1:D:127:GLU:OE2	1:D:131:GLU:OE1	2.34	0.45
1:B:263:VAL:HB	1:B:320:LEU:HD23	1.99	0.44
1:D:136:MET:CE	1:D:166:THR:CA	2.85	0.44
1:A:235:ARG:HG3	1:A:235:ARG:NH1	2.32	0.44
1:B:70:VAL:HG21	1:B:110:SER:HA	1.99	0.44
1:C:275:THR:HG21	2:C:670:HOH:O	2.16	0.44
1:B:145:GLU:OE1	1:C:330:PRO:HB2	2.17	0.44
1:D:78:LYS:C	1:D:78:LYS:CD	2.91	0.44
1:A:149:VAL:HG13	1:A:149:VAL:O	2.18	0.44
1:B:67:PHE:CD1	1:B:73:LEU:HD13	2.53	0.44
1:B:58:ILE:HD13	1:B:102:LEU:HB2	2.00	0.44
1:C:139:TYR:CG	1:C:325:GLY:HA2	2.53	0.44
1:D:221:MET:SD	1:D:259:ILE:HD12	2.58	0.44
1:A:54:GLY:O	1:A:98:ILE:HD13	2.17	0.44
1:D:29:CYS:O	1:D:30:ARG:HG3	2.18	0.44
1:A:4:ARG:HD3	1:A:162:VAL:CG1	2.48	0.43
1:A:257:HIS:HE1	1:B:248:TYR:OH	2.00	0.43
1:D:200:TRP:CE2	1:D:204:GLU:HG3	2.53	0.43
1:D:86:SER:O	1:D:87:THR:C	2.62	0.43
1:A:210:THR:HG23	1:B:303:LYS:HG2	2.00	0.43
1:C:292:CYS:SG	1:D:292:CYS:HB3	2.59	0.43
1:D:58:ILE:HD13	1:D:102:LEU:HB2	2.00	0.43
1:C:248:TYR:CE1	1:D:222:GLN:HG3	2.53	0.43
1:B:92:VAL:O	1:B:96:VAL:HG23	2.18	0.43
1:D:135:LYS:HB2	1:D:135:LYS:HE3	1.77	0.43
1:D:245:ILE:HG13	1:D:308:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:O	1:B:42:LEU:HB2	2.19	0.42
1:C:142:GLU:HG3	2:C:592:HOH:O	2.20	0.42
1:C:305:TYR:HB3	1:D:212:ILE:HG22	2.01	0.42
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.88	0.42
1:A:70:VAL:O	1:A:73:LEU:HB3	2.20	0.42
1:A:245:ILE:HG13	1:A:308:ALA:O	2.20	0.42
1:D:76:HIS:O	1:D:79:LYS:N	2.53	0.42
1:D:235:ARG:HH21	1:D:279:VAL:HG22	1.85	0.42
1:A:223:LYS:HE2	2:A:661:HOH:O	2.19	0.42
1:C:220:VAL:HG13	1:C:226:VAL:HG23	2.01	0.42
1:A:22:GLU:HG2	1:A:23:LYS:CG	2.38	0.42
1:A:128:GLU:C	1:A:131:GLU:HG2	2.45	0.42
1:A:282:GLU:HG3	1:A:284:ARG:NH1	2.35	0.42
1:B:243:ASN:O	1:B:244:LYS:C	2.63	0.42
1:B:23:LYS:HD3	1:B:25:GLU:CG	2.42	0.41
1:A:257:HIS:CE1	1:B:248:TYR:OH	2.73	0.41
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.74	0.41
1:B:75:GLU:HG2	1:B:79:LYS:HE2	2.03	0.41
1:C:257:HIS:HE1	2:C:467:HOH:O	2.03	0.41
1:A:67:PHE:CE2	1:A:73:LEU:HA	2.55	0.41
1:A:223:LYS:CE	2:A:661:HOH:O	2.67	0.41
1:C:191:LEU:HD11	1:C:288:GLU:CD	2.45	0.41
1:D:245:ILE:HG13	1:D:245:ILE:H	1.66	0.41
1:B:23:LYS:CD	1:B:25:GLU:OE2	2.66	0.41
1:D:101:ALA:HA	1:D:121:GLU:HG2	2.03	0.41
1:A:183:VAL:O	1:A:209:VAL:HA	2.20	0.41
1:A:217:VAL:HG21	1:A:250:VAL:HG22	2.03	0.41
1:A:245:ILE:HG13	1:A:308:ALA:C	2.46	0.41
1:B:221:MET:SD	1:B:253:VAL:HG12	2.61	0.41
1:B:284:ARG:HA	1:B:284:ARG:HD3	1.89	0.41
1:C:113:GLU:HA	1:C:116:GLU:HG2	2.03	0.41
1:D:3:LEU:HD13	2:D:488:HOH:O	2.21	0.41
1:A:22:GLU:HB2	1:B:296:GLN:OE1	2.21	0.41
1:D:88:ARG:NH2	2:D:620:HOH:O	2.45	0.41
1:D:32:VAL:O	1:D:32:VAL:HG12	2.21	0.40
1:A:134:ARG:HH11	1:A:134:ARG:HD2	1.76	0.40
1:C:295:ARG:HG3	1:C:295:ARG:NH1	2.36	0.40
1:A:245:ILE:HG21	1:A:307:PRO:HG2	2.03	0.40
1:B:41:LYS:HD2	1:B:43:ALA:HB2	2.04	0.40
1:D:136:MET:HE3	1:D:166:THR:HA	1.98	0.40
1:A:32:VAL:HG23	2:A:479:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PRO:HB3	1:A:129:ASP:CG	2.45	0.40
1:A:292:CYS:CB	1:B:292:CYS:HG	2.26	0.40
1:B:174:ALA:O	1:B:177:GLN:HB2	2.22	0.40
1:B:221:MET:SD	1:B:259:ILE:HD12	2.61	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	338/351 (96%)	326 (96%)	11 (3%)	1 (0%)	36	29
1	B	338/351 (96%)	328 (97%)	10 (3%)	0	100	100
1	C	338/351 (96%)	327 (97%)	11 (3%)	0	100	100
1	D	338/351 (96%)	324 (96%)	14 (4%)	0	100	100
All	All	1352/1404 (96%)	1305 (96%)	46 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	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	281/290 (97%)	260 (92%)	21 (8%)	12	6
1	B	281/290 (97%)	267 (95%)	14 (5%)	22	14
1	C	281/290 (97%)	267 (95%)	14 (5%)	22	14
1	D	281/290 (97%)	267 (95%)	14 (5%)	22	14
All	All	1124/1160 (97%)	1061 (94%)	63 (6%)	19	11

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	ASP
1	A	14	LEU
1	A	19	LYS
1	A	20	LEU
1	A	23	LYS
1	A	32	VAL
1	A	44	VAL
1	A	64	GLU
1	A	99	GLU
1	A	116	GLU
1	A	144	LEU
1	A	151	LEU
1	A	180	GLU
1	A	182	ARG
1	A	191	LEU
1	A	211	LEU
1	A	228	LYS
1	A	235	ARG
1	A	245	ILE
1	A	315	GLU
1	B	12	LEU
1	B	24	LEU
1	B	35	LEU
1	B	60	LEU
1	B	78	LYS
1	B	94	LEU
1	B	119	LEU
1	B	180	GLU
1	B	220	VAL
1	B	234	ASP
1	B	287	GLU
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	292	CYS
1	B	339	LEU
1	C	3	LEU
1	C	41	LYS
1	C	45	ARG
1	C	72	GLU
1	C	77	LEU
1	C	94	LEU
1	C	145	GLU
1	C	211	LEU
1	C	213	THR
1	C	220	VAL
1	C	234	ASP
1	C	295	ARG
1	C	323	GLU
1	C	339	LEU
1	D	2	SER
1	D	3	LEU
1	D	12	LEU
1	D	22	GLU
1	D	82	ASP
1	D	90	THR
1	D	107	LYS
1	D	112	GLU
1	D	135	LYS
1	D	168	LEU
1	D	202	LEU
1	D	245	ILE
1	D	287	GLU
1	D	294	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	257	HIS
1	B	334	ASN
1	C	256	HIS
1	D	76	HIS
1	D	258	ASN
1	D	301	ASN
1	D	316	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/351 (96%)	-0.24	8 (2%) 59 63	16, 28, 57, 81	0
1	B	340/351 (96%)	-0.55	4 (1%) 76 79	15, 24, 39, 55	0
1	C	340/351 (96%)	-0.45	2 (0%) 85 87	17, 25, 42, 57	0
1	D	340/351 (96%)	-0.14	4 (1%) 76 79	17, 30, 61, 82	0
All	All	1360/1404 (96%)	-0.34	18 (1%) 75 78	15, 26, 53, 82	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	4.9
1	A	32	VAL	4.0
1	D	68	ALA	3.3
1	A	65	ARG	3.2
1	A	90	THR	3.0
1	D	31	ASN	2.7
1	A	69	ASP	2.6
1	D	78	LYS	2.6
1	A	70	VAL	2.4
1	C	91	ALA	2.4
1	A	67	PHE	2.3
1	B	293	GLY	2.3
1	C	10	ASP	2.2
1	A	116	GLU	2.1
1	B	103	ASN	2.1
1	D	90	THR	2.1
1	B	65	ARG	2.1
1	B	66	GLU	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 oligosaccharides 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.