Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:46 PM GMT

PDB ID	:	1V4G
Title	:	Crystal Structure of gamma-Glutamylcysteine Synthetase from Escherichia coli B
Authors	:	Hibi, T.; Nii, H.; Nakatsu, T.; Kato, H.; Hiratake, J.; Oda, J.
Deposited on	:	2003-11-13
Resolution	:	2.50 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:

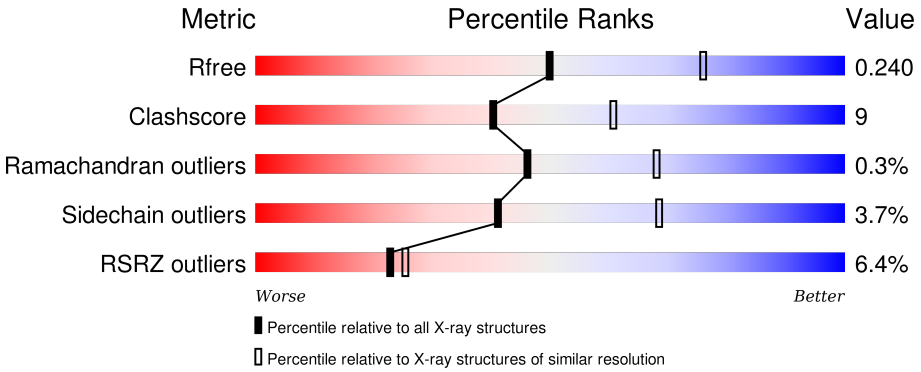
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	518	83% 14%
1	B	518	7% 78% 19%
1	C	518	8% 71% 25%
1	D	518	9% 75% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16214 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4021	2554	689	760	18			
1	B	505	Total	C	N	O	S	0	0	0
			3951	2517	670	746	18			
1	C	509	Total	C	N	O	S	0	0	0
			4010	2551	682	759	18			
1	D	501	Total	C	N	O	S	0	0	0
			3919	2497	667	737	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	FME	MET	MODIFIED RESIDUE	UNP P0A6W9
A	106	SER	CYS	ENGINEERED	UNP P0A6W9
A	164	SER	CYS	ENGINEERED	UNP P0A6W9
A	205	SER	CYS	ENGINEERED	UNP P0A6W9
A	223	SER	CYS	ENGINEERED	UNP P0A6W9
B	1	FME	MET	MODIFIED RESIDUE	UNP P0A6W9
B	106	SER	CYS	ENGINEERED	UNP P0A6W9
B	164	SER	CYS	ENGINEERED	UNP P0A6W9
B	205	SER	CYS	ENGINEERED	UNP P0A6W9
B	223	SER	CYS	ENGINEERED	UNP P0A6W9
C	1	FME	MET	MODIFIED RESIDUE	UNP P0A6W9
C	106	SER	CYS	ENGINEERED	UNP P0A6W9
C	164	SER	CYS	ENGINEERED	UNP P0A6W9
C	205	SER	CYS	ENGINEERED	UNP P0A6W9
C	223	SER	CYS	ENGINEERED	UNP P0A6W9
D	1	FME	MET	MODIFIED RESIDUE	UNP P0A6W9
D	106	SER	CYS	ENGINEERED	UNP P0A6W9
D	164	SER	CYS	ENGINEERED	UNP P0A6W9
D	205	SER	CYS	ENGINEERED	UNP P0A6W9
D	223	SER	CYS	ENGINEERED	UNP P0A6W9

- Molecule 2 is water.

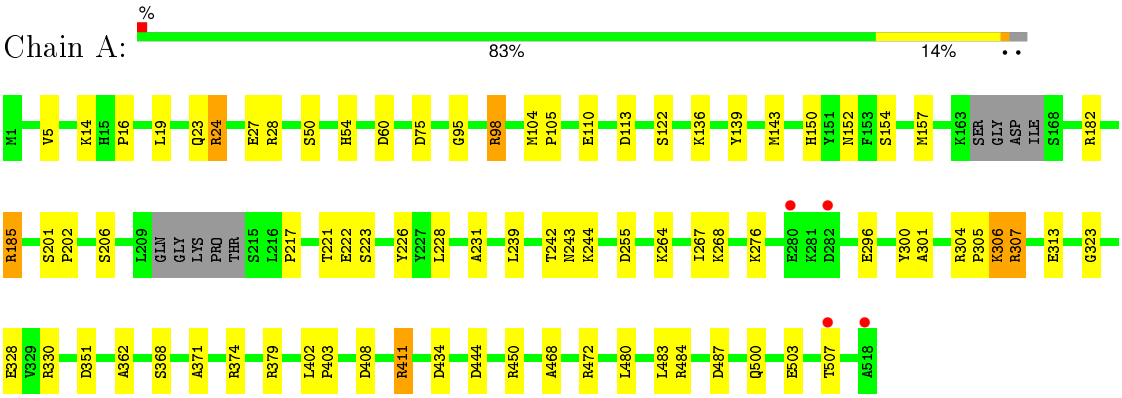
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	159	Total O 159 159	0	0
2	B	58	Total O 58 58	0	0
2	C	38	Total O 38 38	0	0
2	D	58	Total O 58 58	0	0

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.

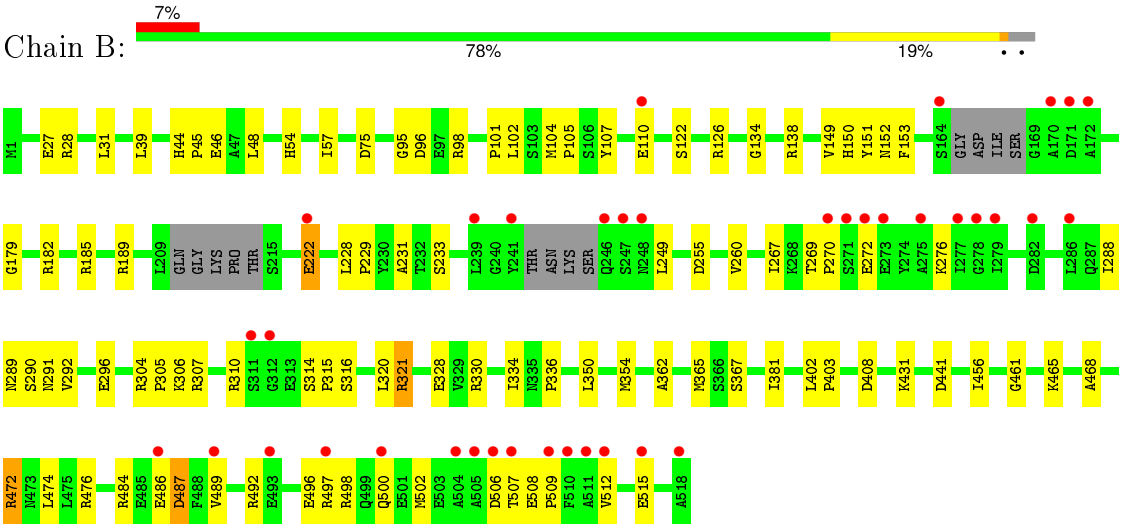
- Molecule 1: Glutamate–cysteine ligase

Chain A:



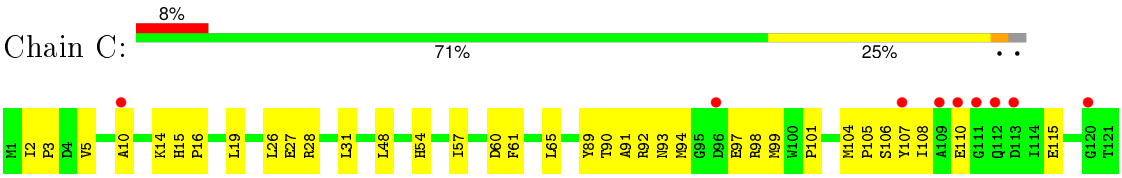
- Molecule 1: Glutamate–cysteine ligase

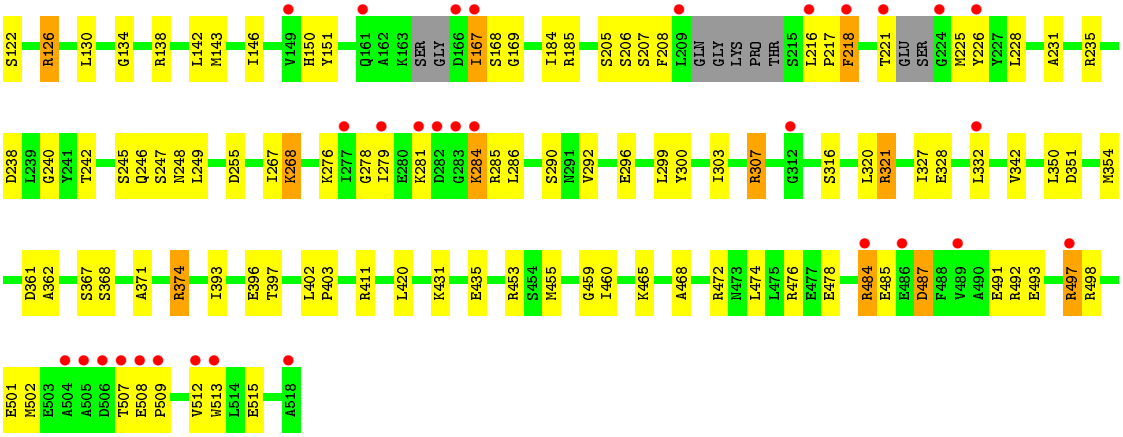
Chain B:



- Molecule 1: Glutamate–cysteine ligase

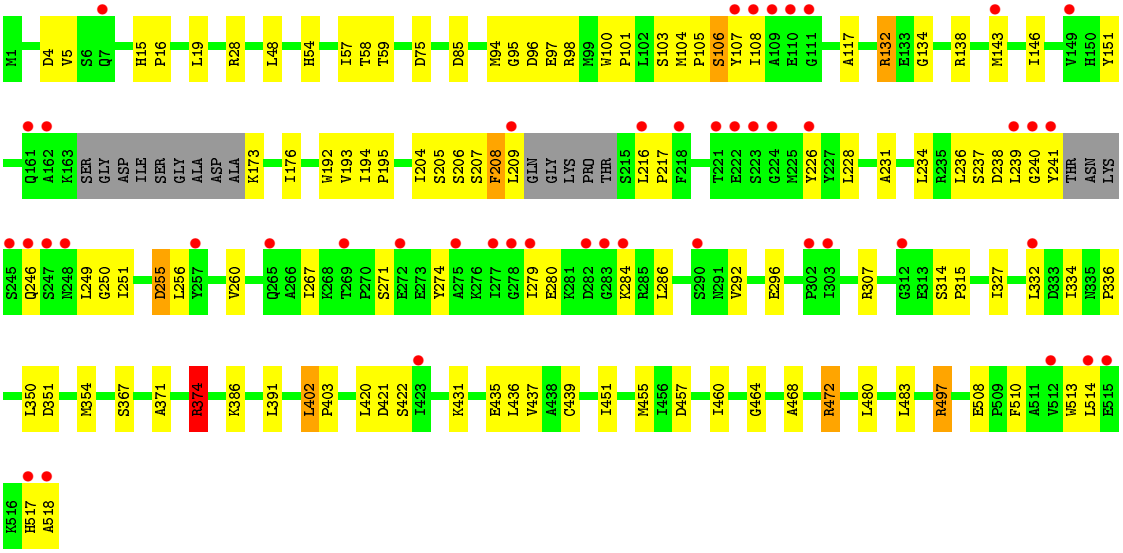
Chain C:





- Molecule 1: Glutamate–cysteine ligase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	326.82Å 326.82Å 104.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.50) 99.9 (39.91-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.206 , 0.236 0.212 , 0.240	Depositor DCC
R_{free} test set	7235 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.5	EDS
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 144145 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16214	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: FME

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	1.08	2/4098 (0.0%)	1.04	10/5546 (0.2%)
1	B	0.95	0/4029	1.00	9/5460 (0.2%)
1	C	0.94	0/4086	1.00	7/5531 (0.1%)
1	D	0.96	1/3997 (0.0%)	1.02	10/5418 (0.2%)
All	All	0.98	3/16210 (0.0%)	1.01	36/21955 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	SER	CB-OG	-5.84	1.34	1.42
1	D	193	VAL	CB-CG2	-5.25	1.41	1.52
1	A	450	ARG	CZ-NH1	-5.18	1.26	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	321	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	113	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	444	ASP	CB-CG-OD2	7.95	125.46	118.30
1	A	185	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	255	ASP	CB-CG-OD2	7.56	125.10	118.30
1	D	374	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	361	ASP	CB-CG-OD2	7.07	124.66	118.30
1	C	307	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	75	ASP	CB-CG-OD2	6.98	124.58	118.30
1	D	96	ASP	CB-CG-OD2	6.88	124.49	118.30
1	C	255	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	238	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	487	ASP	CB-CG-OD2	6.29	123.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	330	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	60	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	60	ASP	CB-CG-OD2	6.13	123.81	118.30
1	D	255	ASP	CB-CG-OD2	6.10	123.79	118.30
1	D	457	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	434	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	255	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	75	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	487	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	321	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	B	441	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	96	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	421	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	132	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	4	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	185	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	75	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	457	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	B	487	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	408	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	85	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4021	0	3939	46	0
1	B	3951	0	3822	58	0
1	C	4010	0	3901	98	0
1	D	3919	0	3782	72	0
2	A	159	0	0	4	0
2	B	58	0	0	2	0
2	C	38	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	58	0	0	0	0
All	All	16214	0	15444	273	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 9.

All (273) 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:167:ILE:O	1:C:167:ILE:HG13	1.49	1.12
1:C:281:LYS:HB2	1:C:286:LEU:HD11	1.35	1.04
1:C:367:SER:HB2	2:C:541:HOH:O	1.70	0.91
1:D:204:ILE:CD1	1:D:239:LEU:HD21	2.09	0.83
1:D:105:PRO:HG2	1:D:208:PHE:CE1	2.13	0.82
1:D:134:GLY:O	1:D:138:ARG:HG3	1.79	0.82
1:C:497:ARG:O	1:C:501:GLU:HG2	1.79	0.82
1:D:204:ILE:HD13	1:D:239:LEU:HD21	1.60	0.81
1:C:218:PHE:CD2	1:C:226:TYR:HB3	2.16	0.80
1:A:244:LYS:HD2	2:A:641:HOH:O	1.82	0.80
1:C:143:MET:HG3	1:C:242:THR:CG2	2.14	0.78
1:B:152:ASN:ND2	1:B:328:GLU:HG3	1.98	0.77
1:C:167:ILE:O	1:C:167:ILE:CG1	2.34	0.75
1:C:91:ALA:HA	1:C:94:MET:HE3	1.67	0.75
1:D:204:ILE:HD11	1:D:209:LEU:HD21	1.68	0.74
1:D:105:PRO:HG2	1:D:208:PHE:HE1	1.52	0.74
1:C:431:LYS:O	1:C:435:GLU:HG3	1.88	0.73
1:C:218:PHE:CE2	1:C:226:TYR:HB3	2.23	0.73
1:A:157:MET:HE2	1:A:157:MET:HA	1.72	0.72
1:D:402:LEU:HB3	1:D:403:PRO:HD3	1.72	0.71
1:B:492:ARG:O	1:B:496:GLU:HG2	1.91	0.70
1:B:484:ARG:HG3	1:B:487:ASP:OD2	1.92	0.70
1:D:451:ILE:O	1:D:455:MET:HG3	1.92	0.69
1:A:152:ASN:ND2	1:A:328:GLU:HG3	2.07	0.69
1:D:271:SER:HB3	1:D:274:TYR:HB2	1.73	0.69
1:A:221:THR:HG22	1:A:223:SER:H	1.58	0.68
1:C:92:ARG:HG3	1:C:476:ARG:HG2	1.73	0.68
1:C:134:GLY:O	1:C:138:ARG:HG3	1.95	0.67
1:B:152:ASN:HD21	1:B:328:GLU:HG3	1.59	0.67
1:C:143:MET:HG3	1:C:242:THR:HG21	1.76	0.67
1:D:204:ILE:HD13	1:D:239:LEU:CD2	2.25	0.66
1:A:157:MET:HA	1:A:157:MET:CE	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HB2	1:C:218:PHE:HD1	1.59	0.66
1:B:107:TYR:OH	1:B:465:LYS:HE2	1.96	0.65
1:C:281:LYS:CB	1:C:286:LEU:HD11	2.21	0.64
1:B:267:ILE:HD11	1:B:296:GLU:CG	2.28	0.64
1:D:246:GLN:HB3	1:D:249:LEU:HD12	1.79	0.64
1:B:267:ILE:HD11	1:B:296:GLU:HG3	1.80	0.63
1:C:108:ILE:HG22	1:C:142:LEU:CD1	2.29	0.63
1:C:108:ILE:HG22	1:C:142:LEU:HD11	1.81	0.63
1:D:256:LEU:O	1:D:260:VAL:HG23	1.99	0.63
1:C:354:MET:CE	1:C:354:MET:HA	2.29	0.62
1:A:143:MET:HE1	1:A:239:LEU:O	2.00	0.62
1:C:31:LEU:HD23	1:C:65:LEU:HD13	1.82	0.62
1:C:91:ALA:HA	1:C:94:MET:CE	2.30	0.61
1:D:250:GLY:HA2	1:D:367:SER:OG	1.99	0.61
1:C:5:VAL:O	1:C:5:VAL:HG12	2.01	0.61
1:D:431:LYS:HE3	1:D:435:GLU:OE2	2.01	0.61
1:B:122:SER:O	1:B:126:ARG:HG3	2.01	0.60
1:A:143:MET:CE	1:A:239:LEU:O	2.50	0.60
1:A:305:PRO:O	1:A:306:LYS:HG2	2.01	0.60
1:C:279:ILE:O	1:C:279:ILE:HG22	2.02	0.60
1:C:249:LEU:HD21	1:C:292:VAL:HG11	1.84	0.60
1:C:397:THR:HG23	2:C:539:HOH:O	2.02	0.59
1:C:185:ARG:NH1	1:C:362:ALA:O	2.35	0.59
1:A:243:ASN:HB3	1:A:300:TYR:HB2	1.83	0.59
1:D:143:MET:HG3	1:D:240:GLY:O	2.03	0.59
1:B:31:LEU:HD22	1:B:39:LEU:HD11	1.84	0.58
1:A:206:SER:HB3	1:A:226:TYR:CE1	2.39	0.57
1:C:94:MET:O	1:C:97:GLU:HB2	2.04	0.57
1:C:91:ALA:HB2	1:C:99:MET:CE	2.34	0.57
1:A:122:SER:HB3	1:A:503:GLU:HG3	1.86	0.57
1:B:289:ASN:OD1	1:B:291:ASN:HB2	2.04	0.57
1:A:152:ASN:HD21	1:A:328:GLU:HG3	1.70	0.56
1:C:90:THR:O	1:C:94:MET:HE2	2.05	0.56
1:D:249:LEU:HD21	1:D:292:VAL:HG21	1.86	0.56
1:B:508:GLU:CB	1:B:509:PRO:HD2	2.36	0.56
1:C:484:ARG:O	1:C:487:ASP:N	2.37	0.56
1:D:100:TRP:CH2	1:D:464:GLY:HA3	2.41	0.56
1:D:204:ILE:CD1	1:D:209:LEU:HD21	2.36	0.55
1:C:515:GLU:HG2	1:C:515:GLU:O	2.06	0.55
1:C:281:LYS:HB2	1:C:286:LEU:CD1	2.23	0.55
1:B:101:PRO:HD3	1:B:468:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:472:ARG:NH2	2.38	0.54
1:D:371:ALA:O	1:D:374:ARG:HB2	2.07	0.54
1:D:314:SER:HB2	1:D:315:PRO:CD	2.38	0.54
1:C:474:LEU:O	1:C:478:GLU:HG3	2.08	0.54
1:B:498:ARG:O	1:B:502:MET:HG3	2.07	0.54
1:B:27:GLU:HB2	1:B:150:HIS:HB2	1.89	0.54
1:B:512:VAL:O	1:B:515:GLU:HB3	2.08	0.54
1:B:229:PRO:HD2	2:B:524:HOH:O	2.08	0.53
1:D:194:ILE:HB	1:D:195:PRO:HD3	1.89	0.53
1:C:228:LEU:HB2	1:C:231:ALA:HB2	1.89	0.53
1:C:245:SER:HA	1:C:300:TYR:HB3	1.90	0.53
1:D:19:LEU:HD13	1:D:420:LEU:HD13	1.91	0.53
1:C:332:LEU:HD11	1:C:350:LEU:HD11	1.90	0.53
1:D:436:LEU:O	1:D:439:CYS:HB2	2.09	0.53
1:B:95:GLY:O	1:B:472:ARG:NH2	2.40	0.53
1:A:14:LYS:C	1:A:16:PRO:HD3	2.29	0.53
1:B:46:GLU:HG2	1:B:492:ARG:NH2	2.24	0.53
1:B:472:ARG:O	1:B:476:ARG:HG3	2.09	0.53
1:C:19:LEU:HD13	1:C:420:LEU:HD21	1.90	0.52
1:C:151:TYR:OH	1:C:351:ASP:OD1	2.27	0.52
1:B:486:GLU:O	1:B:489:VAL:HG22	2.08	0.52
1:D:209:LEU:HD23	1:D:239:LEU:HD11	1.91	0.52
1:A:402:LEU:HB3	1:A:403:PRO:HD3	1.92	0.52
1:C:105:PRO:HB3	1:C:108:ILE:HD12	1.90	0.52
1:C:221:THR:OG1	1:C:225:MET:HB3	2.10	0.52
1:D:241:TYR:CD1	1:D:241:TYR:O	2.63	0.52
1:C:106:SER:O	1:C:107:TYR:HB2	2.10	0.52
1:C:245:SER:O	1:C:248:ASN:HB3	2.10	0.52
1:C:104:MET:HE2	1:C:235:ARG:HB2	1.92	0.52
1:B:267:ILE:CG2	1:B:267:ILE:O	2.58	0.51
1:C:246:GLN:HA	1:C:299:LEU:HD11	1.92	0.51
1:B:134:GLY:O	1:B:138:ARG:HG3	2.10	0.51
1:D:510:PHE:O	1:D:513:TRP:HB3	2.10	0.51
1:C:54:HIS:HB3	1:C:57:ILE:O	2.10	0.51
1:B:486:GLU:O	1:B:489:VAL:CG2	2.58	0.51
1:D:236:LEU:O	1:D:241:TYR:CE2	2.63	0.51
1:C:455:MET:O	1:C:459:GLY:HA2	2.11	0.51
1:C:15:HIS:N	1:C:16:PRO:HD3	2.25	0.51
1:D:431:LYS:O	1:D:435:GLU:HG3	2.09	0.51
1:A:185:ARG:NH1	1:A:362:ALA:O	2.44	0.51
1:C:216:LEU:C	1:C:218:PHE:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:THR:OG1	1:B:508:GLU:N	2.44	0.50
1:D:15:HIS:N	1:D:16:PRO:HD3	2.24	0.50
1:C:216:LEU:HB2	1:C:218:PHE:CD1	2.45	0.50
1:C:14:LYS:C	1:C:16:PRO:HD3	2.32	0.50
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.77	0.50
1:D:19:LEU:CD1	1:D:420:LEU:HD13	2.42	0.50
1:C:130:LEU:HD21	1:C:285:ARG:HG2	1.93	0.49
1:B:189:ARG:HD2	1:B:365:MET:HE2	1.95	0.49
1:C:267:ILE:HG21	1:C:296:GLU:HG2	1.95	0.49
1:C:509:PRO:HG2	1:C:512:VAL:HG23	1.93	0.49
1:C:101:PRO:HD3	1:C:468:ALA:HB2	1.93	0.49
1:C:110:GLU:HA	1:C:142:LEU:HD22	1.95	0.49
1:B:228:LEU:HB2	1:B:231:ALA:HB2	1.93	0.49
1:D:104:MET:HE2	1:D:146:ILE:HG12	1.93	0.49
1:B:496:GLU:HA	1:B:496:GLU:OE1	2.13	0.49
1:B:296:GLU:OE1	1:B:315:PRO:HD2	2.13	0.49
1:D:58:THR:OG1	1:D:59:THR:N	2.45	0.48
1:D:5:VAL:HG12	1:D:5:VAL:O	2.13	0.48
1:D:267:ILE:HD11	1:D:296:GLU:HG2	1.95	0.48
1:A:307:ARG:HD2	1:A:323:GLY:O	2.13	0.48
1:C:327:ILE:HG22	1:C:328:GLU:N	2.28	0.48
1:D:206:SER:HA	1:D:209:LEU:HD12	1.95	0.48
1:A:371:ALA:O	1:A:374:ARG:HB2	2.13	0.48
1:D:206:SER:HB3	1:D:226:TYR:HE1	1.77	0.48
1:A:50:SER:O	1:A:54:HIS:HB2	2.13	0.48
1:B:486:GLU:C	1:B:489:VAL:HG22	2.34	0.48
1:B:54:HIS:HB3	1:B:57:ILE:O	2.13	0.48
1:B:461:GLY:O	1:B:465:LYS:HG3	2.14	0.48
1:C:296:GLU:OE2	1:C:316:SER:OG	2.23	0.48
1:C:89:TYR:CE1	1:C:93:ASN:ND2	2.82	0.48
1:B:267:ILE:HG22	1:B:267:ILE:O	2.14	0.47
1:C:393:ILE:O	1:C:396:GLU:HB2	2.14	0.47
1:D:117:ALA:HB3	1:D:132:ARG:CD	2.44	0.47
1:C:146:ILE:HD12	1:C:240:GLY:O	2.14	0.47
1:B:272:GLU:O	1:B:276:LYS:HG3	2.14	0.47
1:C:216:LEU:HD12	1:C:218:PHE:HE1	1.78	0.47
1:B:304:ARG:HD3	2:B:531:HOH:O	2.14	0.47
1:A:507:THR:HG21	1:B:222:GLU:HG3	1.95	0.47
1:C:90:THR:HG22	1:C:94:MET:CE	2.44	0.47
1:A:301:ALA:O	1:A:330:ARG:HD2	2.14	0.47
1:A:304:ARG:HG3	1:A:305:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LEU:O	1:D:241:TYR:HE2	1.97	0.47
1:B:102:LEU:HD23	1:B:336:PRO:HB3	1.95	0.47
1:A:264:LYS:HB3	2:A:653:HOH:O	2.14	0.47
1:C:268:LYS:HE3	1:C:268:LYS:HB3	1.58	0.47
1:D:204:ILE:HG23	1:D:234:LEU:HD12	1.96	0.46
1:A:267:ILE:HD11	1:A:296:GLU:HG2	1.97	0.46
1:A:139:TYR:HB3	1:A:242:THR:HB	1.96	0.46
1:D:205:SER:O	1:D:208:PHE:HB2	2.15	0.46
1:C:26:LEU:HD13	1:C:342:VAL:HG11	1.96	0.46
1:C:206:SER:C	1:C:208:PHE:H	2.18	0.46
1:B:104:MET:HA	1:B:105:PRO:HD3	1.81	0.45
1:C:508:GLU:HG3	1:C:513:TRP:HB2	1.98	0.45
1:B:48:LEU:HD13	1:B:57:ILE:HG21	1.99	0.45
1:D:228:LEU:HB2	1:D:231:ALA:HB2	1.98	0.45
1:A:27:GLU:HB2	1:A:150:HIS:HB2	1.99	0.45
1:A:157:MET:CE	1:A:157:MET:CA	2.93	0.45
1:B:267:ILE:HD11	1:B:296:GLU:HG2	1.97	0.45
1:C:27:GLU:HB2	1:C:150:HIS:HB2	1.99	0.45
1:C:498:ARG:O	1:C:502:MET:HG3	2.16	0.45
1:A:306:LYS:HE2	1:A:328:GLU:OE1	2.17	0.45
1:D:279:ILE:O	1:D:286:LEU:N	2.48	0.45
1:A:139:TYR:HB3	1:A:242:THR:CB	2.47	0.45
1:C:354:MET:HE1	1:C:354:MET:HA	1.99	0.45
1:D:48:LEU:O	1:D:54:HIS:CD2	2.70	0.45
1:D:391:LEU:HD11	1:D:402:LEU:HD12	1.98	0.45
1:C:48:LEU:O	1:C:54:HIS:CD2	2.69	0.45
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.81	0.45
1:C:321:ARG:NH1	1:C:321:ARG:HG2	2.32	0.45
1:D:151:TYR:OH	1:D:351:ASP:OD1	2.34	0.45
1:D:517:HIS:CD2	1:D:518:ALA:N	2.84	0.44
1:C:245:SER:OG	1:C:248:ASN:HB2	2.17	0.44
1:A:307:ARG:NH2	2:A:569:HOH:O	2.50	0.44
1:D:334:ILE:O	1:D:336:PRO:HD3	2.18	0.44
1:A:408:ASP:OD1	1:A:411:ARG:NH1	2.50	0.44
1:D:105:PRO:CG	1:D:208:PHE:CE1	2.94	0.44
1:B:288:ILE:HG22	1:B:289:ASN:HD22	1.82	0.44
1:A:201:SER:N	1:A:202:PRO:HD3	2.32	0.44
1:D:480:LEU:HB3	1:D:483:LEU:O	2.17	0.44
1:B:48:LEU:O	1:B:54:HIS:CD2	2.71	0.44
1:D:327:ILE:HD11	1:D:354:MET:SD	2.57	0.44
1:B:249:LEU:HD21	1:B:292:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:PHE:CE2	1:D:514:LEU:HD11	2.53	0.44
1:C:327:ILE:CG2	1:C:328:GLU:N	2.80	0.43
1:B:44:HIS:HA	1:B:45:PRO:HD3	1.84	0.43
1:C:19:LEU:HA	1:C:19:LEU:HD23	1.88	0.43
1:C:205:SER:O	1:C:208:PHE:HB2	2.18	0.43
1:C:225:MET:SD	1:C:460:ILE:HG13	2.58	0.43
1:B:151:TYR:CD2	1:B:350:LEU:HD13	2.53	0.43
1:C:168:SER:O	1:C:169:GLY:C	2.56	0.43
1:A:104:MET:HA	1:A:105:PRO:HD3	1.83	0.43
1:B:179:GLY:O	1:B:182:ARG:HB3	2.18	0.43
1:C:320:LEU:HD12	1:C:320:LEU:HA	1.91	0.43
1:C:107:TYR:CZ	1:C:465:LYS:HE3	2.54	0.43
1:B:149:VAL:HG23	1:B:334:ILE:HD13	2.01	0.43
1:C:276:LYS:C	1:C:278:GLY:N	2.71	0.43
1:C:402:LEU:HB3	1:C:403:PRO:HD3	2.01	0.43
1:A:221:THR:HG22	1:A:222:GLU:N	2.33	0.43
1:C:107:TYR:CE2	1:C:465:LYS:HE3	2.54	0.43
1:C:2:ILE:HA	1:C:3:PRO:HD3	1.93	0.43
1:A:480:LEU:HB3	1:A:483:LEU:O	2.19	0.42
1:D:497:ARG:O	1:D:497:ARG:HG2	2.19	0.42
1:D:508:GLU:CD	1:D:508:GLU:H	2.22	0.42
1:D:173:LYS:O	1:D:176:ILE:HB	2.18	0.42
1:C:143:MET:HG3	1:C:242:THR:HG23	1.95	0.42
1:C:279:ILE:HD11	1:C:290:SER:HB3	2.01	0.42
1:D:451:ILE:HD12	1:D:451:ILE:HA	1.88	0.42
1:D:95:GLY:O	1:D:472:ARG:NH2	2.52	0.42
1:D:280:GLU:HA	1:D:284:LYS:O	2.20	0.42
1:B:267:ILE:CD1	1:B:296:GLU:HG3	2.49	0.42
1:C:371:ALA:O	1:C:374:ARG:HB2	2.20	0.42
1:A:24:ARG:HG3	2:A:535:HOH:O	2.19	0.42
1:A:24:ARG:NH2	1:A:351:ASP:OD2	2.41	0.42
1:B:233:SER:O	1:B:381:ILE:HG23	2.20	0.42
1:D:101:PRO:HD3	1:D:468:ALA:HB2	2.02	0.42
1:B:260:VAL:HG13	1:B:316:SER:HB2	2.02	0.42
1:D:249:LEU:O	1:D:250:GLY:C	2.58	0.42
1:C:10:ALA:O	1:C:14:LYS:HG3	2.19	0.42
1:B:269:THR:HA	1:B:270:PRO:HD3	1.81	0.42
1:A:23:GLN:HB2	1:A:154:SER:OG	2.20	0.42
1:C:91:ALA:HB2	1:C:99:MET:HE1	2.02	0.42
1:B:486:GLU:CA	1:B:489:VAL:HG22	2.50	0.42
1:D:94:MET:O	1:D:97:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:MET:O	1:D:94:MET:HG3	2.20	0.41
1:A:5:VAL:HG12	1:A:5:VAL:O	2.20	0.41
1:C:491:GLU:O	1:C:492:ARG:C	2.56	0.41
1:C:122:SER:O	1:C:126:ARG:HB2	2.20	0.41
1:C:284:LYS:HD2	1:C:286:LEU:HD23	2.03	0.41
1:B:402:LEU:N	1:B:403:PRO:CD	2.83	0.41
1:D:107:TYR:C	1:D:108:ILE:HG13	2.41	0.41
1:C:493:GLU:HB3	1:C:497:ARG:NH2	2.35	0.41
1:B:305:PRO:O	1:B:306:LYS:HG2	2.20	0.41
1:A:304:ARG:NH2	1:A:330:ARG:HH21	2.18	0.41
1:B:185:ARG:NH1	1:B:362:ALA:O	2.54	0.41
1:C:184:ILE:HG12	1:C:303:ILE:HG12	2.03	0.41
1:A:268:LYS:HG3	1:A:268:LYS:O	2.19	0.41
1:D:117:ALA:HB3	1:D:132:ARG:HD3	2.01	0.41
1:A:201:SER:N	1:A:202:PRO:CD	2.84	0.41
1:B:153:PHE:CE2	1:B:354:MET:HB3	2.56	0.41
1:C:281:LYS:HB3	1:C:286:LEU:HD21	2.03	0.41
1:D:143:MET:SD	1:D:208:PHE:CE2	3.14	0.41
1:C:279:ILE:O	1:C:279:ILE:CG2	2.68	0.41
1:A:221:THR:CG2	1:A:222:GLU:N	2.84	0.41
1:C:296:GLU:HG3	2:C:531:HOH:O	2.20	0.41
1:D:105:PRO:HB2	1:D:108:ILE:HD12	2.03	0.40
1:C:507:THR:OG1	1:C:508:GLU:N	2.54	0.40
1:D:332:LEU:HD11	1:D:350:LEU:HD11	2.03	0.40
1:A:228:LEU:HB2	1:A:231:ALA:HB2	2.02	0.40
1:C:206:SER:O	1:C:208:PHE:N	2.54	0.40
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.82	0.40
1:D:237:SER:C	1:D:239:LEU:H	2.23	0.40
1:B:497:ARG:HA	1:B:500:GLN:OE1	2.20	0.40
1:D:314:SER:HB2	1:D:315:PRO:HD2	2.02	0.40
1:D:54:HIS:HB3	1:D:57:ILE:O	2.22	0.40
1:B:314:SER:HB2	1:B:315:PRO:HD2	2.04	0.40
1:D:192:TRP:C	1:D:195:PRO:HD2	2.42	0.40
1:A:98:ARG:HG3	1:A:468:ALA:HB1	2.03	0.40
1:D:106:SER:HB2	1:D:460:ILE:HG22	2.04	0.40
1:D:216:LEU:HA	1:D:217:PRO:HD3	1.85	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	503/518 (97%)	488 (97%)	14 (3%)	1 (0%)	52 75
1	B	497/518 (96%)	481 (97%)	16 (3%)	0	100 100
1	C	501/518 (97%)	474 (95%)	23 (5%)	4 (1%)	24 41
1	D	493/518 (95%)	465 (94%)	27 (6%)	1 (0%)	52 75
All	All	1994/2072 (96%)	1908 (96%)	80 (4%)	6 (0%)	46 68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	485	GLU
1	C	207	SER
1	C	218	PHE
1	C	217	PRO
1	D	238	ASP
1	A	217	PRO

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	419/433 (97%)	406 (97%)	13 (3%)	47 75
1	B	403/433 (93%)	389 (96%)	14 (4%)	43 70
1	C	412/433 (95%)	395 (96%)	17 (4%)	37 63
1	D	398/433 (92%)	382 (96%)	16 (4%)	38 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1632/1732 (94%)	1572 (96%)	60 (4%)	41 68

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	28	ARG
1	A	98	ARG
1	A	110	GLU
1	A	136	LYS
1	A	182	ARG
1	A	276	LYS
1	A	306	LYS
1	A	307	ARG
1	A	313	GLU
1	A	411	ARG
1	A	484	ARG
1	A	500	GLN
1	B	28	ARG
1	B	98	ARG
1	B	110	GLU
1	B	222	GLU
1	B	290	SER
1	B	307	ARG
1	B	310	ARG
1	B	321	ARG
1	B	367	SER
1	B	431	LYS
1	B	456	ILE
1	B	472	ARG
1	B	474	LEU
1	B	506	ASP
1	C	28	ARG
1	C	61	PHE
1	C	98	ARG
1	C	115	GLU
1	C	126	ARG
1	C	167	ILE
1	C	247	SER
1	C	268	LYS
1	C	284	LYS
1	C	307	ARG

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Mol	Chain	Res	Type
1	C	368	SER
1	C	374	ARG
1	C	411	ARG
1	C	453	ARG
1	C	472	ARG
1	C	484	ARG
1	C	497	ARG
1	D	28	ARG
1	D	98	ARG
1	D	103	SER
1	D	106	SER
1	D	207	SER
1	D	208	PHE
1	D	251	ILE
1	D	255	ASP
1	D	307	ARG
1	D	374	ARG
1	D	386	LYS
1	D	402	LEU
1	D	422	SER
1	D	437	VAL
1	D	472	ARG
1	D	497	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	A	152	ASN
1	B	152	ASN
1	B	404	GLN
1	C	93	ASN
1	C	150	HIS
1	C	152	ASN
1	C	418	GLN
1	D	152	ASN
1	D	404	GLN
1	D	517	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.04	1 (12%)	6,9,11	4.17	2 (33%)
1	FME	B	1	1	6,7,10	0.60	0	4,7,11	1.01	0
1	FME	C	1	1	8,9,10	1.05	1 (12%)	6,9,11	2.92	2 (33%)
1	FME	D	1	1	6,7,10	1.59	1 (16%)	4,7,11	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
1	FME	B	1	1	-	0/4/6/11	0/0/0/0
1	FME	C	1	1	-	1/6/9/11	0/0/0/0
1	FME	D	1	1	-	0/4/6/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	FME	CB-CA	-3.46	1.50	1.53
1	C	1	FME	CA-N	2.48	1.49	1.46
1	A	1	FME	CA-N	2.58	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	O1-CN-N	-9.07	111.69	124.76
1	C	1	FME	O1-CN-N	-5.67	116.59	124.76
1	C	1	FME	CA-N-CN	4.22	129.32	122.82
1	A	1	FME	CA-N-CN	4.47	129.70	122.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

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

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	508/518 (98%)	-0.12	4 (0%) 87 89	9, 23, 44, 56	0
1	B	504/518 (97%)	0.15	38 (7%) 17 19	17, 34, 55, 87	0
1	C	508/518 (98%)	0.29	40 (7%) 15 17	21, 39, 57, 84	0
1	D	500/518 (96%)	0.28	47 (9%) 11 11	16, 35, 54, 85	0
All	All	2020/2072 (97%)	0.15	129 (6%) 23 25	9, 33, 54, 87	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	ASN	6.5
1	C	507	THR	6.0
1	D	279	ILE	5.7
1	D	111	GLY	5.7
1	C	216	LEU	5.7
1	B	164	SER	5.7
1	C	110	GLU	5.5
1	C	109	ALA	5.4
1	D	278	GLY	5.3
1	D	518	ALA	5.1
1	D	110	GLU	5.0
1	C	282	ASP	4.9
1	D	239	LEU	4.8
1	B	172	ALA	4.8
1	C	111	GLY	4.6
1	D	109	ALA	4.5
1	A	282	ASP	4.4
1	D	209	LEU	4.4
1	B	247	SER	4.3
1	B	239	LEU	4.3
1	D	283	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	245	SER	4.1
1	B	500	GLN	4.1
1	B	512	VAL	4.1
1	C	509	PRO	4.0
1	B	504	ALA	3.9
1	C	518	ALA	3.9
1	B	275	ALA	3.8
1	B	509	PRO	3.8
1	C	283	GLY	3.7
1	D	282	ASP	3.7
1	B	277	ILE	3.7
1	D	275	ALA	3.6
1	D	107	TYR	3.6
1	D	512	VAL	3.6
1	D	223	SER	3.5
1	D	222	GLU	3.5
1	B	171	ASP	3.5
1	D	257	TYR	3.5
1	B	312	GLY	3.5
1	B	507	THR	3.5
1	B	506	ASP	3.4
1	B	515	GLU	3.4
1	D	277	ILE	3.4
1	B	511	ALA	3.4
1	C	504	ALA	3.4
1	C	279	ILE	3.4
1	B	246	GLN	3.3
1	B	273	GLU	3.3
1	D	247	SER	3.3
1	B	272	GLU	3.3
1	C	512	VAL	3.2
1	D	272	GLU	3.2
1	C	484	ARG	3.2
1	C	284	LYS	3.2
1	C	161	GLN	3.2
1	B	489	VAL	3.2
1	B	518	ALA	3.1
1	B	311	SER	3.1
1	C	489	VAL	3.1
1	C	107	TYR	3.0
1	C	221	THR	3.0
1	B	505	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	281	LYS	3.0
1	C	226	TYR	3.0
1	C	224	GLY	2.9
1	D	224	GLY	2.9
1	C	508	GLU	2.9
1	C	166	ASP	2.9
1	C	120	GLY	2.9
1	C	486	GLU	2.8
1	C	218	PHE	2.8
1	D	161	GLN	2.7
1	C	209	LEU	2.7
1	D	312	GLY	2.7
1	D	515	GLU	2.7
1	B	248	ASN	2.7
1	C	513	TRP	2.7
1	B	493	GLU	2.6
1	B	241	TYR	2.6
1	B	278	GLY	2.6
1	D	240	GLY	2.6
1	B	497	ARG	2.6
1	C	312	GLY	2.6
1	C	112	GLN	2.6
1	C	167	ILE	2.5
1	B	279	ILE	2.5
1	D	265	GLN	2.5
1	B	286	LEU	2.5
1	C	497	ARG	2.5
1	B	486	GLU	2.4
1	A	507	THR	2.4
1	B	282	ASP	2.4
1	D	149	VAL	2.4
1	D	226	TYR	2.3
1	B	222	GLU	2.3
1	B	270	PRO	2.3
1	D	143	MET	2.3
1	C	332	LEU	2.3
1	D	241	TYR	2.3
1	D	332	LEU	2.3
1	D	162	ALA	2.3
1	D	302	PRO	2.3
1	C	10	ALA	2.3
1	C	149	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	518	ALA	2.2
1	D	246	GLN	2.2
1	D	221	THR	2.2
1	D	290	SER	2.2
1	D	514	LEU	2.2
1	C	277	ILE	2.2
1	D	269	THR	2.2
1	B	510	PHE	2.1
1	C	113	ASP	2.1
1	D	517	HIS	2.1
1	B	170	ALA	2.1
1	D	108	ILE	2.1
1	A	280	GLU	2.1
1	C	505	ALA	2.1
1	B	110	GLU	2.1
1	D	218	PHE	2.1
1	B	271	SER	2.1
1	D	423	ILE	2.1
1	D	216	LEU	2.1
1	D	284	LYS	2.1
1	C	506	ASP	2.1
1	D	303	ILE	2.0
1	C	96	ASP	2.0
1	D	7	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	FME	B	1	8/11	0.95	0.14	-	32,36,40,46	0
1	FME	D	1	8/11	0.94	0.14	-	36,38,47,52	0
1	FME	A	1	10/11	0.93	0.11	-	25,37,48,53	0
1	FME	C	1	10/11	0.91	0.12	-	27,36,45,54	0

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.