Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:22 PM GMT

PDB ID	:	4LF3
Title	:	Inhibitory Mechanism of an Allosteric Antibody Targeting the Glucagon Receptor
Authors	:	Murray, J.M.; Mukund, S.
Deposited on	:	2013-06-26
Resolution	:	2.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

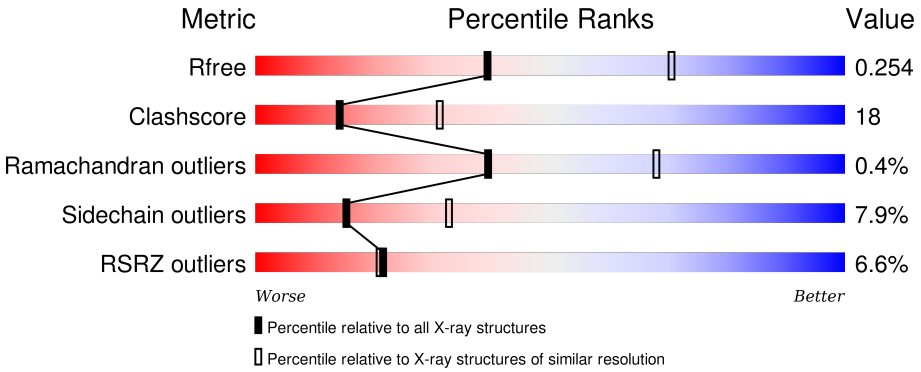
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	11% 58% 41%
1	D	214	3% 58% 36% 5%
2	B	231	6% 70% 27%
2	E	231	3% 65% 31%
3	C	95	15% 61% 38%

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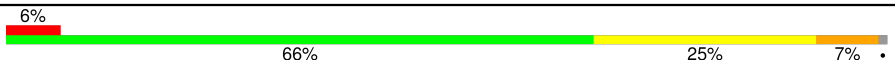
Mol	Chain	Length	Quality of chain
3	F	95	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8470 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			
1	D	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	231	Total	C	N	O	S	0	0	0
			1758	1109	298	343	8			
2	E	231	Total	C	N	O	S	0	0	0
			1756	1108	298	342	8			

- Molecule 3 is a protein called Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			798	512	144	134	8			
3	F	94	Total	C	N	O	S	0	0	0
			790	507	143	133	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	SER	GLY	ENGINEERED MUTATION	UNP P47871
F	40	SER	GLY	ENGINEERED MUTATION	UNP P47871

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		

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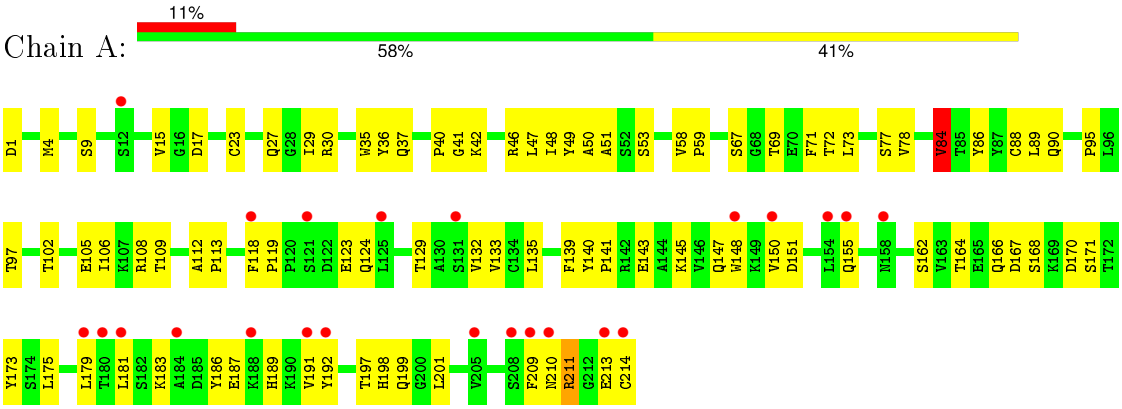
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	19	Total O 19 19	0	0
4	C	6	Total O 6 6	0	0
4	D	21	Total O 21 21	0	0
4	E	37	Total O 37 37	0	0
4	F	7	Total O 7 7	0	0

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.

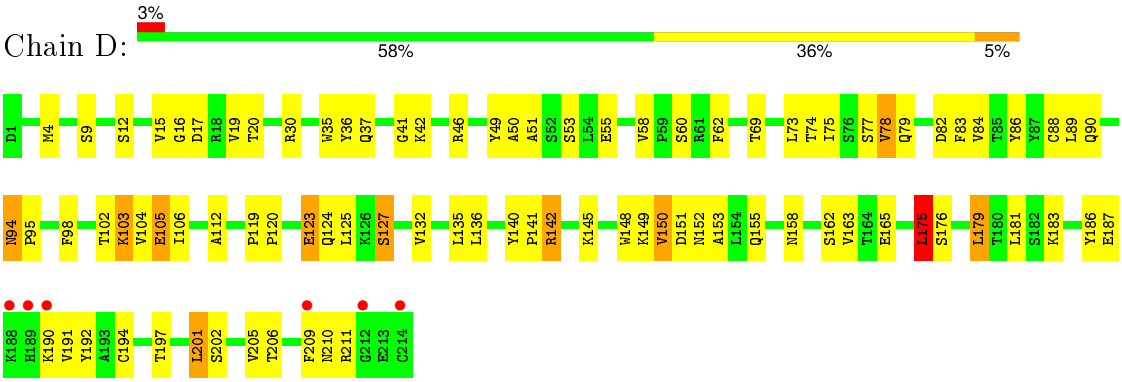
- Molecule 1: Fab heavy chain

Chain A:



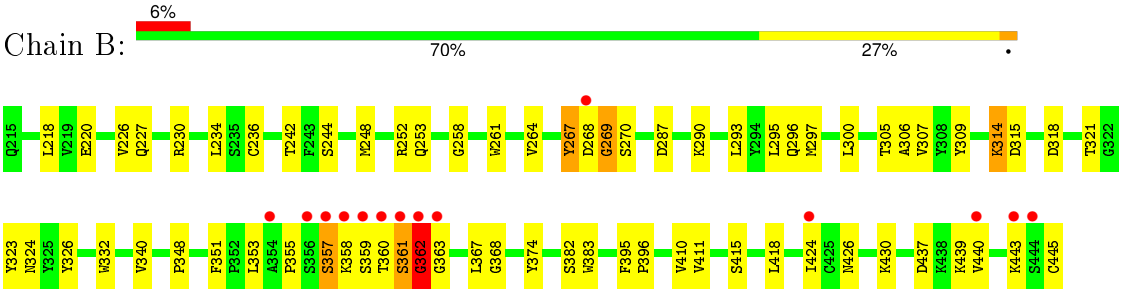
- Molecule 1: Fab heavy chain

Chain D:



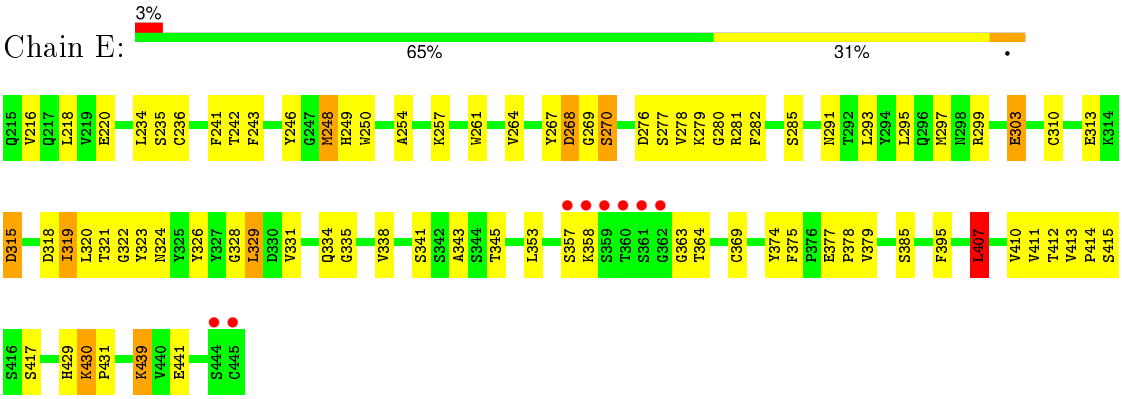
- Molecule 2: Fab light chain

Chain B:



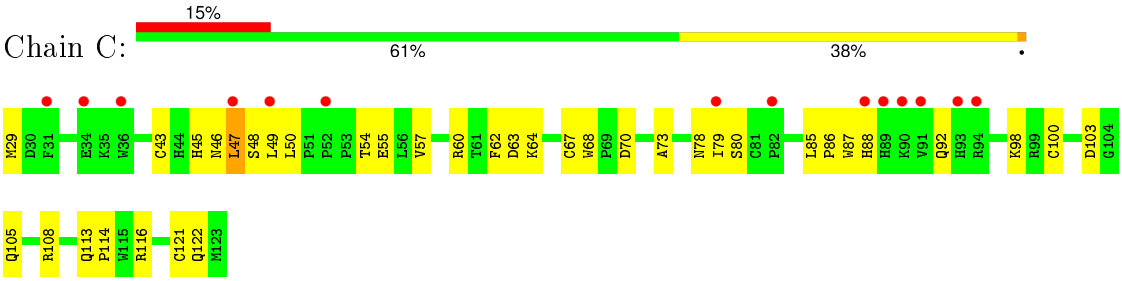
- Molecule 2: Fab light chain

Chain E:



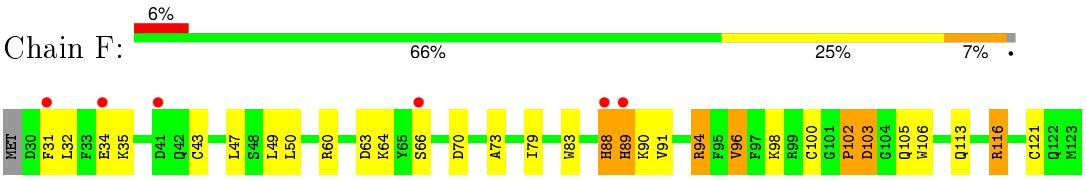
- Molecule 3: Glucagon receptor

Chain C:



- Molecule 3: Glucagon receptor

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.93Å 62.78Å 116.43Å 90.00° 106.04° 90.00°	Depositor
Resolution (Å)	55.95 – 2.73 55.95 – 2.73	Depositor EDS
% Data completeness (in resolution range)	92.2 (55.95-2.73) 92.2 (55.95-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.209 , 0.264 0.203 , 0.254	Depositor DCC
R_{free} test set	1787 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 35924 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8470	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.54	1/1666 (0.1%)	0.73	0/2259
1	D	0.51	0/1666	0.76	3/2259 (0.1%)
2	B	0.51	0/1802	0.80	2/2453 (0.1%)
2	E	0.55	0/1800	0.70	1/2450 (0.0%)
3	C	0.49	0/832	0.72	1/1136 (0.1%)
3	F	0.50	0/824	0.64	0/1126
All	All	0.52	1/8590 (0.0%)	0.74	7/11683 (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
3	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	PRO	N-CD	5.35	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	94	ASN	C-N-CD	-9.12	100.53	120.60
2	B	362	GLY	N-CA-C	6.37	129.03	113.10
1	D	95	PRO	N-CA-C	-6.37	95.54	112.10
2	B	269	GLY	N-CA-C	-5.61	99.08	113.10
2	E	407	LEU	CA-CB-CG	5.57	128.11	115.30
1	D	175	LEU	CA-CB-CG	5.44	127.82	115.30
3	C	47	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	94	ASN	Peptide
3	F	103	ASP	Peptide

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	1633	0	1590	67	0
1	D	1633	0	1590	53	0
2	B	1758	0	1705	62	0
2	E	1756	0	1700	72	0
3	C	798	0	740	26	0
3	F	790	0	731	33	0
4	A	12	0	0	2	0
4	B	19	0	0	3	0
4	C	6	0	0	0	0
4	D	21	0	0	1	0
4	E	37	0	0	7	0
4	F	7	0	0	1	0
All	All	8470	0	8056	297	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 18.

All (297) 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)
2:E:321:THR:HG23	2:E:323:TYR:H	1.23	1.02
3:F:66:SER:HB2	3:F:79:ILE:HD11	1.47	0.96
2:B:318:ASP:HB3	2:B:321:THR:HG22	1.45	0.95
2:B:357:SER:HB2	2:B:359:SER:H	1.28	0.95
3:F:103:ASP:HB3	3:F:105:GLN:H	1.31	0.95
3:F:50:LEU:HB2	3:F:60:ARG:HH12	1.32	0.94
2:B:357:SER:HB2	2:B:359:SER:N	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:ASP:HB3	2:E:321:THR:HG22	1.50	0.91
3:F:63:ASP:OD2	3:F:98:LYS:NZ	2.04	0.91
3:F:50:LEU:HB2	3:F:60:ARG:NH1	1.86	0.91
2:E:243:PHE:HE1	2:E:248:MET:HE3	1.39	0.86
1:D:123:GLU:OE1	1:D:123:GLU:N	2.10	0.84
2:B:426:ASN:ND2	2:B:437:ASP:OD1	2.11	0.83
1:A:113:PRO:HB3	1:A:139:PHE:HB3	1.63	0.81
2:E:243:PHE:HE1	2:E:248:MET:CE	1.96	0.79
1:A:135:LEU:HD22	2:B:410:VAL:HG11	1.63	0.78
3:C:63:ASP:O	3:C:64:LYS:HB2	1.83	0.78
2:E:220:GLU:OE2	2:E:335:GLY:N	2.17	0.77
2:B:321:THR:HG23	2:B:323:TYR:H	1.47	0.77
3:C:79:ILE:HG22	3:C:80:SER:O	1.85	0.77
2:E:322:GLY:O	3:F:116:ARG:NH2	2.20	0.75
3:F:103:ASP:HB3	3:F:105:GLN:N	2.02	0.74
1:D:190:LYS:HG2	1:D:191:VAL:HG13	1.68	0.74
2:B:227:GLN:H	2:B:230:ARG:HH11	1.37	0.73
3:C:47:LEU:HA	3:C:50:LEU:HD12	1.73	0.71
3:F:98:LYS:HD3	3:F:106:TRP:CE3	2.27	0.70
1:D:120:PRO:HD3	1:D:132:VAL:HG12	1.74	0.70
2:B:314:LYS:HE3	4:B:502:HOH:O	1.93	0.69
1:A:150:VAL:HG12	1:A:155:GLN:NE2	2.06	0.69
2:B:357:SER:CB	2:B:359:SER:H	2.03	0.69
2:E:297:MET:HE1	2:E:338:VAL:HG21	1.73	0.69
2:E:318:ASP:HB3	2:E:321:THR:CG2	2.23	0.68
3:F:43:CYS:O	3:F:47:LEU:HB2	1.94	0.67
2:E:269:GLY:CA	4:E:501:HOH:O	2.42	0.67
1:A:41:GLY:C	1:A:42:LYS:HD2	2.15	0.67
2:B:357:SER:CB	2:B:358:LYS:HA	2.22	0.66
3:C:47:LEU:HA	3:C:50:LEU:CD1	2.25	0.66
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.31	0.65
1:A:186:TYR:HA	1:A:192:TYR:OH	1.97	0.65
3:C:103:ASP:OD2	3:C:105:GLN:HG3	1.97	0.64
2:B:227:GLN:HB2	2:B:230:ARG:HD3	1.78	0.64
2:E:318:ASP:CB	2:E:321:THR:HG22	2.27	0.64
2:E:254:ALA:HB3	2:E:257:LYS:HG3	1.80	0.64
2:B:318:ASP:CB	2:B:321:THR:HG22	2.23	0.63
2:B:318:ASP:HB3	2:B:321:THR:CG2	2.25	0.63
3:F:31:PHE:HA	3:F:34:GLU:HB2	1.80	0.63
2:B:357:SER:HB2	2:B:358:LYS:CA	2.29	0.62
2:E:269:GLY:HA3	4:E:501:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:O	1:D:55:GLU:HG3	2.00	0.62
1:D:191:VAL:HG12	1:D:210:ASN:HB3	1.82	0.62
1:A:46:ARG:HD3	1:A:49:TYR:HB3	1.81	0.62
2:E:243:PHE:CE1	2:E:248:MET:CE	2.83	0.61
2:B:270:SER:O	3:C:108:ARG:NH2	2.33	0.61
2:E:248:MET:HB3	2:E:293:LEU:HD22	1.81	0.61
1:D:187:GLU:O	1:D:211:ARG:NH1	2.34	0.60
1:A:113:PRO:CB	1:A:139:PHE:HB3	2.30	0.60
1:A:118:PHE:CD2	2:B:353:LEU:HB3	2.36	0.60
2:E:430:LYS:N	2:E:431:PRO:CD	2.63	0.60
2:B:218:LEU:HD22	2:B:236:CYS:SG	2.41	0.60
2:B:297:MET:HB3	2:B:300:LEU:HD21	1.84	0.59
3:F:88:HIS:CE1	3:F:89:HIS:HD2	2.20	0.59
1:D:119:PRO:HB3	1:D:209:PHE:CE1	2.38	0.59
2:E:321:THR:HG23	2:E:323:TYR:N	2.06	0.59
1:A:50:ALA:O	1:A:51:ALA:HB3	2.02	0.59
2:E:276:ASP:OD1	2:E:279:LYS:HD2	2.02	0.58
3:F:66:SER:CB	3:F:79:ILE:HD11	2.28	0.58
2:E:268:ASP:CB	2:E:269:GLY:HA2	2.32	0.58
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.39	0.58
1:A:186:TYR:CD1	1:A:192:TYR:CZ	2.92	0.58
3:F:47:LEU:HD12	3:F:50:LEU:CD1	2.34	0.58
2:B:227:GLN:H	2:B:230:ARG:NH1	2.01	0.58
1:D:74:THR:HG23	4:D:302:HOH:O	2.03	0.57
3:C:63:ASP:HB2	3:C:114:PRO:HB3	1.87	0.57
1:A:112:ALA:HB1	1:A:201:LEU:HD12	1.86	0.57
2:B:355:PRO:HD3	2:B:367:LEU:HB3	1.85	0.57
1:A:145:LYS:HB2	1:A:197:THR:HB	1.86	0.57
1:D:119:PRO:HB3	1:D:209:PHE:CZ	2.40	0.57
2:E:261:TRP:HZ2	2:E:264:VAL:HG12	1.68	0.57
1:D:145:LYS:HD3	1:D:197:THR:HB	1.86	0.57
2:B:230:ARG:HG2	4:B:504:HOH:O	2.03	0.57
1:A:191:VAL:HG12	1:A:210:ASN:HB3	1.87	0.57
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.39	0.57
2:E:268:ASP:OD1	2:E:269:GLY:HA2	2.05	0.56
1:D:145:LYS:HD2	1:D:145:LYS:N	2.20	0.56
3:C:43:CYS:SG	3:C:47:LEU:HD13	2.46	0.56
1:A:183:LYS:O	1:A:187:GLU:HB2	2.06	0.56
1:A:112:ALA:HB1	1:A:201:LEU:CD1	2.36	0.55
1:D:158:ASN:ND2	1:D:179:LEU:HD11	2.21	0.55
2:E:357:SER:O	2:E:358:LYS:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HG2	1:A:129:THR:O	2.06	0.55
3:C:62:PHE:CE2	3:C:64:LYS:HA	2.42	0.55
1:A:162:SER:OG	2:B:396:PRO:HG2	2.07	0.55
3:F:88:HIS:CE1	3:F:89:HIS:CD2	2.94	0.55
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.88	0.55
1:D:9:SER:O	1:D:102:THR:HA	2.07	0.55
2:B:236:CYS:HB3	2:B:293:LEU:HB3	1.89	0.55
2:E:413:VAL:HB	2:E:414:PRO:HD2	1.88	0.55
1:D:12:SER:HA	1:D:105:GLU:O	2.08	0.54
1:D:37:GLN:HG3	1:D:86:TYR:CE2	2.42	0.54
1:A:118:PHE:HB2	1:A:133:VAL:HG22	1.88	0.54
2:B:267:TYR:OH	2:B:315:ASP:OD1	2.26	0.54
1:A:42:LYS:HD2	1:A:42:LYS:N	2.22	0.54
1:A:67:SER:HA	1:A:71:PHE:CE1	2.43	0.54
3:F:73:ALA:HA	3:F:100:CYS:SG	2.47	0.54
1:D:125:LEU:O	1:D:183:LYS:HD2	2.08	0.54
2:E:243:PHE:CD2	2:E:291:ASN:HA	2.43	0.54
2:B:363:GLY:N	2:B:415:SER:HB3	2.23	0.54
2:E:319:ILE:O	4:E:537:HOH:O	2.18	0.54
1:D:35:TRP:CZ3	1:D:88:CYS:HB3	2.43	0.54
2:B:362:GLY:HA3	2:B:415:SER:OG	2.06	0.53
3:C:43:CYS:HA	3:C:46:ASN:HB2	1.91	0.53
1:D:112:ALA:HB1	1:D:201:LEU:CD1	2.39	0.53
2:E:414:PRO:HG2	2:E:417:SER:HB2	1.90	0.52
2:E:269:GLY:HA2	4:E:501:HOH:O	2.07	0.52
1:D:120:PRO:HD3	1:D:132:VAL:CG1	2.38	0.52
1:D:35:TRP:CE2	1:D:73:LEU:HB2	2.45	0.52
2:E:280:GLY:O	2:E:299:ARG:NH2	2.42	0.52
1:A:164:THR:HG23	2:B:395:PHE:CD1	2.45	0.52
1:A:118:PHE:HB2	1:A:133:VAL:CG2	2.40	0.52
1:D:41:GLY:O	1:D:42:LYS:HD2	2.10	0.52
1:D:50:ALA:O	1:D:51:ALA:HB3	2.10	0.51
1:D:151:ASP:OD1	1:D:190:LYS:HB3	2.10	0.51
1:A:210:ASN:N	1:A:210:ASN:OD1	2.43	0.51
3:F:63:ASP:O	3:F:64:LYS:HB2	2.10	0.51
1:A:151:ASP:OD2	1:A:189:HIS:ND1	2.44	0.51
2:B:382:SER:OG	2:B:426:ASN:HB2	2.10	0.51
2:E:281:ARG:HG2	2:E:299:ARG:CZ	2.41	0.51
1:A:58:VAL:HG13	1:A:59:PRO:HD2	1.93	0.51
1:D:16:GLY:HA2	1:D:77:SER:HB2	1.93	0.51
1:A:166:GLN:HB2	1:A:173:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:VAL:HG12	2:B:411:VAL:N	2.26	0.50
3:C:49:LEU:O	3:C:50:LEU:HG	2.10	0.50
1:D:140:TYR:CG	1:D:141:PRO:HA	2.46	0.50
1:A:89:LEU:HD12	1:A:97:THR:O	2.11	0.50
2:E:326:TYR:OH	3:F:113:GLN:HB3	2.12	0.50
1:D:83:PHE:CD2	1:D:104:VAL:HG12	2.47	0.50
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.46	0.50
3:F:50:LEU:CB	3:F:60:ARG:HH12	2.15	0.49
2:E:268:ASP:HB2	2:E:270:SER:N	2.27	0.49
2:B:357:SER:HB2	2:B:358:LYS:C	2.30	0.49
3:F:98:LYS:HD3	3:F:106:TRP:CZ3	2.48	0.49
2:E:411:VAL:HG22	2:E:412:THR:N	2.28	0.49
2:B:357:SER:HB2	2:B:358:LYS:HA	1.90	0.49
2:E:236:CYS:HB3	2:E:293:LEU:HB3	1.94	0.49
3:C:73:ALA:HA	3:C:100:CYS:SG	2.53	0.49
2:E:278:VAL:HB	2:E:282:PHE:CG	2.48	0.49
3:C:49:LEU:HD12	3:C:49:LEU:O	2.11	0.49
2:B:287:ASP:OD2	2:B:290:LYS:HE3	2.13	0.49
1:A:113:PRO:HB3	1:A:139:PHE:CD2	2.48	0.48
1:A:49:TYR:O	1:A:53:SER:HB2	2.13	0.48
3:F:91:VAL:HA	3:F:94:ARG:HH11	1.77	0.48
1:A:36:TYR:CE2	1:A:46:ARG:HB2	2.48	0.48
1:A:167:ASP:OD1	1:A:168:SER:N	2.46	0.48
2:E:285:SER:O	2:E:293:LEU:HD12	2.14	0.48
2:E:358:LYS:O	2:E:358:LYS:HG2	2.14	0.48
3:C:45:HIS:O	3:C:48:SER:OG	2.31	0.48
2:E:343:ALA:HB3	2:E:375:PHE:CZ	2.49	0.48
1:A:4:MET:HE3	1:A:23:CYS:SG	2.54	0.47
3:F:96:VAL:HG22	3:F:121:CYS:SG	2.55	0.47
3:C:43:CYS:SG	3:C:47:LEU:CD1	3.03	0.47
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.49	0.47
2:B:424:ILE:HG12	2:B:439:LYS:HA	1.97	0.47
3:C:67:CYS:O	3:C:79:ILE:HD11	2.14	0.47
2:E:313:GLU:HG3	2:E:328:GLY:O	2.13	0.47
2:B:360:THR:O	2:B:362:GLY:N	2.47	0.47
3:F:113:GLN:O	3:F:113:GLN:HG2	2.14	0.47
1:D:186:TYR:CD1	1:D:192:TYR:CZ	3.03	0.47
1:A:140:TYR:CG	1:A:141:PRO:HA	2.49	0.47
1:A:113:PRO:HB3	1:A:139:PHE:CB	2.39	0.47
1:A:67:SER:HA	1:A:71:PHE:HE1	1.79	0.47
1:D:49:TYR:CZ	1:D:53:SER:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:395:PHE:O	2:E:407:LEU:HD22	2.14	0.47
1:D:36:TYR:OH	2:E:329:LEU:O	2.21	0.47
3:F:60:ARG:N	3:F:70:ASP:OD1	2.46	0.47
2:E:268:ASP:HB2	2:E:269:GLY:CA	2.44	0.46
3:C:88:HIS:O	3:C:92:GLN:HB3	2.14	0.46
2:B:410:VAL:CG1	2:B:411:VAL:N	2.79	0.46
3:C:47:LEU:CA	3:C:50:LEU:HD12	2.42	0.46
1:D:163:VAL:HG22	1:D:175:LEU:HB2	1.97	0.46
2:E:261:TRP:CZ2	2:E:264:VAL:HG12	2.50	0.46
1:D:175:LEU:C	1:D:175:LEU:HD12	2.36	0.46
2:E:379:VAL:HG12	2:E:429:HIS:CD2	2.50	0.46
1:D:79:GLN:O	1:D:82:ASP:HB2	2.16	0.46
1:D:103:LYS:NZ	1:D:165:GLU:OE2	2.49	0.46
2:E:216:VAL:HG13	2:E:241:PHE:CD1	2.51	0.46
2:E:267:TYR:OH	2:E:315:ASP:OD1	2.34	0.45
1:A:186:TYR:HD1	1:A:192:TYR:CZ	2.33	0.45
2:B:368:GLY:HA2	2:B:383:TRP:CH2	2.50	0.45
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.51	0.45
1:A:164:THR:HG23	2:B:395:PHE:CE1	2.51	0.45
2:E:220:GLU:HA	2:E:235:SER:O	2.17	0.45
2:E:220:GLU:CD	4:E:510:HOH:O	2.55	0.45
1:A:48:ILE:HG23	1:A:53:SER:O	2.16	0.45
1:D:175:LEU:HA	2:E:395:PHE:HE2	1.81	0.45
2:B:332:TRP:CD1	2:B:332:TRP:N	2.83	0.45
1:D:145:LYS:HD2	1:D:145:LYS:H	1.81	0.45
2:E:261:TRP:HZ2	2:E:264:VAL:CG1	2.28	0.45
2:E:364:THR:HG23	2:E:413:VAL:O	2.17	0.45
2:B:439:LYS:HG3	2:B:440:VAL:N	2.31	0.45
2:B:268:ASP:N	2:B:269:GLY:HA2	2.32	0.45
3:F:98:LYS:HB3	3:F:106:TRP:CZ3	2.52	0.45
1:A:9:SER:O	1:A:102:THR:HA	2.17	0.45
1:A:213:GLU:OE2	2:B:443:LYS:HE2	2.17	0.45
2:B:295:LEU:HD12	2:B:295:LEU:HA	1.76	0.45
2:B:226:VAL:O	2:B:340:VAL:HA	2.16	0.45
2:B:253:GLN:HG3	2:B:258:GLY:O	2.16	0.45
3:F:88:HIS:HE1	3:F:89:HIS:HD2	1.64	0.45
3:F:35:LYS:HD2	3:F:83:TRP:HZ3	1.82	0.45
2:E:220:GLU:CG	4:E:510:HOH:O	2.64	0.44
2:E:268:ASP:CB	2:E:269:GLY:CA	2.95	0.44
2:E:430:LYS:N	2:E:431:PRO:HD3	2.31	0.44
2:E:320:LEU:HD21	3:F:32:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:ARG:HB3	3:C:70:ASP:OD1	2.17	0.44
1:A:199:GLN:C	1:A:201:LEU:H	2.19	0.44
2:B:261:TRP:HZ2	2:B:264:VAL:HG12	1.82	0.44
3:F:47:LEU:HA	3:F:50:LEU:HD12	1.98	0.44
3:F:90:LYS:HG2	3:F:94:ARG:HH12	1.82	0.44
2:E:281:ARG:HG2	2:E:299:ARG:NH2	2.32	0.44
1:D:124:GLN:O	1:D:127:SER:OG	2.34	0.44
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.78	0.44
1:A:108:ARG:HD2	1:A:170:ASP:O	2.18	0.44
2:B:363:GLY:O	2:B:415:SER:N	2.46	0.44
3:F:103:ASP:OD2	3:F:105:GLN:HB2	2.17	0.44
1:D:135:LEU:CD2	2:E:410:VAL:HG11	2.47	0.44
2:E:243:PHE:CE1	2:E:248:MET:HE2	2.50	0.43
1:A:124:GLN:HG3	2:B:351:PHE:CE2	2.52	0.43
2:B:360:THR:C	2:B:362:GLY:H	2.21	0.43
2:E:377:GLU:HB3	2:E:378:PRO:HA	2.00	0.43
3:C:87:TRP:NE1	3:C:121:CYS:O	2.44	0.43
2:E:374:TYR:CE2	2:E:379:VAL:HG13	2.53	0.43
2:E:250:TRP:NE1	2:E:295:LEU:HB2	2.32	0.43
2:E:303:GLU:HB2	4:E:505:HOH:O	2.17	0.43
2:E:319:ILE:H	2:E:319:ILE:HG12	1.40	0.43
2:E:363:GLY:O	2:E:415:SER:CB	2.67	0.43
2:B:314:LYS:HG3	2:B:315:ASP:N	2.32	0.43
1:A:72:THR:HG22	4:A:306:HOH:O	2.18	0.43
1:A:151:ASP:CG	1:A:189:HIS:HD1	2.21	0.43
2:E:218:LEU:HA	2:E:218:LEU:HD23	1.71	0.43
2:E:246:TYR:N	2:E:246:TYR:CD1	2.86	0.43
1:D:17:ASP:O	1:D:77:SER:HA	2.19	0.43
1:D:149:LYS:HA	1:D:153:ALA:O	2.19	0.43
3:C:49:LEU:C	3:C:50:LEU:HG	2.39	0.43
2:B:326:TYR:OH	3:C:113:GLN:HB3	2.19	0.43
1:D:89:LEU:HD13	1:D:98:PHE:CE1	2.54	0.43
2:E:345:THR:HA	2:E:375:PHE:O	2.18	0.43
2:E:297:MET:CE	2:E:338:VAL:HG21	2.47	0.42
2:E:353:LEU:HD12	2:E:369:CYS:N	2.34	0.42
3:C:68:TRP:CE2	3:C:98:LYS:HD2	2.53	0.42
1:D:55:GLU:HB2	1:D:58:VAL:HG21	2.00	0.42
2:B:248:MET:HB3	2:B:293:LEU:HD22	2.02	0.42
2:B:269:GLY:HA2	4:B:516:HOH:O	2.18	0.42
1:D:19:VAL:HG23	1:D:78:VAL:HG22	2.01	0.42
1:D:210:ASN:N	1:D:210:ASN:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HB3	1:A:209:PHE:CD2	2.54	0.42
1:A:186:TYR:O	1:A:211:ARG:HD2	2.19	0.42
1:D:205:VAL:HG12	1:D:206:THR:N	2.34	0.42
2:B:318:ASP:OD2	2:B:321:THR:HG22	2.19	0.42
3:F:47:LEU:HG	3:F:60:ARG:HD3	2.01	0.42
1:A:199:GLN:C	1:A:201:LEU:N	2.73	0.42
2:E:343:ALA:HB3	2:E:375:PHE:CE2	2.55	0.42
3:C:85:LEU:HA	3:C:86:PRO:HD3	1.85	0.42
1:D:55:GLU:OE2	1:D:55:GLU:HA	2.19	0.41
1:A:108:ARG:HD3	1:A:171:SER:O	2.18	0.41
1:A:214:CYS:HA	2:B:445:CYS:CB	2.50	0.41
1:D:150:VAL:O	1:D:151:ASP:C	2.56	0.41
2:E:439:LYS:HD3	2:E:441:GLU:CG	2.50	0.41
2:B:305:THR:O	2:B:306:ALA:HB2	2.20	0.41
2:B:252:ARG:HA	2:B:307:VAL:O	2.20	0.41
2:E:243:PHE:CE1	2:E:248:MET:HE3	2.32	0.41
1:A:113:PRO:CA	1:A:139:PHE:HB3	2.48	0.41
3:C:47:LEU:HA	3:C:50:LEU:HD11	2.01	0.41
1:D:41:GLY:C	1:D:42:LYS:HD2	2.41	0.41
2:B:220:GLU:OE1	2:B:309:TYR:HA	2.21	0.41
1:A:17:ASP:O	1:A:77:SER:HA	2.20	0.41
1:D:142:ARG:HH11	1:D:163:VAL:CG1	2.34	0.41
3:C:55:GLU:O	3:C:57:VAL:HG13	2.20	0.41
2:E:249:HIS:O	2:E:310:CYS:HA	2.21	0.41
2:B:348:PRO:HB3	2:B:374:TYR:HB3	2.02	0.41
1:D:20:THR:OG1	1:D:74:THR:HG22	2.20	0.41
2:B:261:TRP:HZ2	2:B:264:VAL:CG1	2.34	0.41
1:A:40:PRO:HD3	1:A:84:VAL:HG12	2.03	0.41
1:A:148:TRP:CE2	1:A:179:LEU:HB2	2.56	0.41
1:D:62:PHE:CE1	1:D:75:ILE:HD13	2.56	0.41
1:A:27:GLN:O	1:A:29:ILE:HG23	2.21	0.41
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.56	0.41
1:A:30:ARG:HD2	4:A:310:HOH:O	2.20	0.41
1:A:36:TYR:O	1:A:86:TYR:HA	2.21	0.40
1:D:148:TRP:HB2	1:D:155:GLN:HB2	2.03	0.40
3:F:105:GLN:HA	4:F:206:HOH:O	2.21	0.40
1:A:198:HIS:CG	1:A:199:GLN:N	2.90	0.40
1:D:4:MET:HE2	1:D:90:GLN:HB2	2.03	0.40
2:B:244:SER:O	2:B:267:TYR:CD1	2.74	0.40
2:E:216:VAL:HG12	2:E:331:VAL:HG21	2.03	0.40
1:D:136:LEU:N	1:D:136:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG12	1:A:155:GLN:HE21	1.82	0.40
2:B:418:LEU:HD12	2:B:418:LEU:N	2.37	0.40
3:F:102:PRO:CD	3:F:103:ASP:H	2.35	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	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	34	62
1	D	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	34	62
2	B	229/231 (99%)	215 (94%)	12 (5%)	2 (1%)	21	47
2	E	229/231 (99%)	220 (96%)	9 (4%)	0	100	100
3	C	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
3	F	92/95 (97%)	87 (95%)	5 (5%)	0	100	100
All	All	1067/1080 (99%)	1018 (95%)	45 (4%)	4 (0%)	39	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	VAL
2	B	362	GLY
2	B	361	SER
1	A	84	VAL

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	187/187 (100%)	172 (92%)	15 (8%)	15 32
1	D	187/187 (100%)	166 (89%)	21 (11%)	7 16
2	B	196/196 (100%)	187 (95%)	9 (5%)	33 62
2	E	195/196 (100%)	178 (91%)	17 (9%)	13 27
3	C	88/88 (100%)	83 (94%)	5 (6%)	25 51
3	F	87/88 (99%)	80 (92%)	7 (8%)	15 32
All	All	940/942 (100%)	866 (92%)	74 (8%)	15 33

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	15	VAL
1	A	69	THR
1	A	78	VAL
1	A	84	VAL
1	A	90	GLN
1	A	105	GLU
1	A	106	ILE
1	A	109	THR
1	A	123	GLU
1	A	143	GLU
1	A	147	GLN
1	A	175	LEU
1	A	181	LEU
1	A	211	ARG
2	B	234	LEU
2	B	242	THR
2	B	267	TYR
2	B	296	GLN
2	B	314	LYS
2	B	324	ASN
2	B	357	SER
2	B	361	SER
2	B	430	LYS
3	C	29	MET
3	C	54	THR

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Mol	Chain	Res	Type
3	C	78	ASN
3	C	116	ARG
3	C	122	GLN
1	D	15	VAL
1	D	30	ARG
1	D	60	SER
1	D	69	THR
1	D	78	VAL
1	D	103	LYS
1	D	105	GLU
1	D	106	ILE
1	D	123	GLU
1	D	127	SER
1	D	142	ARG
1	D	150	VAL
1	D	152	ASN
1	D	162	SER
1	D	175	LEU
1	D	176	SER
1	D	179	LEU
1	D	181	LEU
1	D	194	CYS
1	D	201	LEU
1	D	202	SER
2	E	234	LEU
2	E	242	THR
2	E	248	MET
2	E	268	ASP
2	E	270	SER
2	E	277	SER
2	E	303	GLU
2	E	315	ASP
2	E	319	ILE
2	E	324	ASN
2	E	329	LEU
2	E	334	GLN
2	E	341	SER
2	E	385	SER
2	E	407	LEU
2	E	430	LYS
2	E	439	LYS
3	F	49	LEU

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Mol	Chain	Res	Type
3	F	88	HIS
3	F	89	HIS
3	F	94	ARG
3	F	96	VAL
3	F	102	PRO
3	F	116	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	89	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	214/214 (100%)	0.93	23 (10%) 8 6	23, 59, 119, 149	0
1	D	214/214 (100%)	0.41	6 (2%) 56 59	9, 44, 85, 123	0
2	B	231/231 (100%)	0.62	14 (6%) 25 24	18, 45, 95, 147	0
2	E	231/231 (100%)	0.41	8 (3%) 48 50	14, 36, 82, 141	0
3	C	95/95 (100%)	1.08	14 (14%) 3 3	28, 60, 113, 147	0
3	F	94/95 (98%)	0.68	6 (6%) 23 22	20, 49, 90, 112	0
All	All	1079/1080 (99%)	0.64	71 (6%) 22 21	9, 46, 105, 149	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	359	SER	6.7
1	A	192	TYR	5.4
2	E	360	THR	5.4
2	E	362	GLY	5.3
1	A	154	LEU	5.1
2	E	359	SER	5.0
2	B	358	LYS	4.9
2	B	360	THR	4.7
1	A	188	LYS	4.7
3	C	89	HIS	4.6
3	C	31	PHE	4.5
1	A	180	THR	4.2
1	D	212	GLY	4.0
1	A	214	CYS	4.0
1	A	125	LEU	3.8
2	B	362	GLY	3.6
1	A	208	SER	3.5
3	F	31	PHE	3.5
1	A	209	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	358	LYS	3.3
3	C	82	PRO	3.3
1	D	214	CYS	3.3
1	A	121	SER	3.1
2	B	361	SER	3.1
3	C	88	HIS	3.0
2	E	361	SER	2.9
2	B	357	SER	2.8
1	A	210	ASN	2.8
2	B	363	GLY	2.8
2	E	445	CYS	2.8
3	C	36	TRP	2.7
3	C	79	ILE	2.7
3	C	91	VAL	2.7
3	C	52	PRO	2.7
2	E	357	SER	2.7
2	B	268	ASP	2.6
1	A	213	GLU	2.6
1	D	209	PHE	2.6
2	E	444	SER	2.6
1	A	179	LEU	2.6
2	B	443	LYS	2.6
1	A	150	VAL	2.6
2	B	356	SER	2.6
1	D	188	LYS	2.5
1	A	181	LEU	2.5
3	C	93	HIS	2.4
3	F	88	HIS	2.4
3	F	89	HIS	2.4
1	D	189	HIS	2.4
2	B	424	ILE	2.4
3	F	34	GLU	2.4
3	C	49	LEU	2.3
2	B	354	ALA	2.3
2	B	444	SER	2.3
1	A	155	GLN	2.3
3	C	34	GLU	2.3
3	C	94	ARG	2.3
1	A	118	PHE	2.3
3	F	66	SER	2.3
1	A	191	VAL	2.3
1	A	158	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	440	VAL	2.2
1	A	131	SER	2.2
1	A	184	ALA	2.2
1	A	12	SER	2.2
1	A	148	TRP	2.1
3	C	47	LEU	2.1
3	C	90	LYS	2.1
3	F	41	ASP	2.1
1	D	190	LYS	2.0
1	A	205	VAL	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.