



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:14 AM UTC

PDB ID : 4LF3 / pdb_00004lf3
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

<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

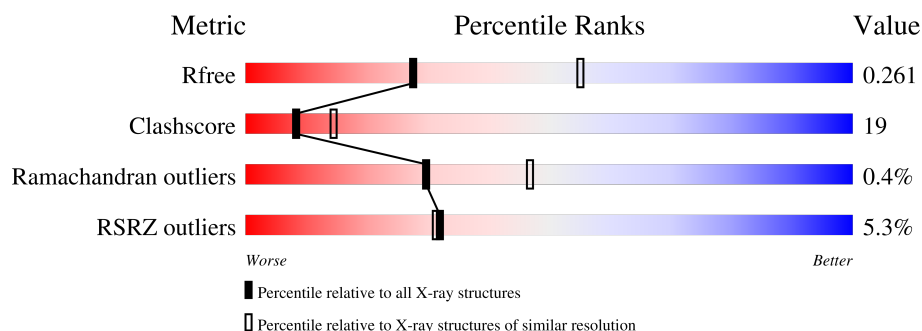
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	214	6% 61%38% .
1	D	214	3% 61%39%
2	B	231	6% 69%30%
2	E	231	4% 65%34% .
3	C	95	12% 59%39% .
3	F	95	3% 62%35% ..

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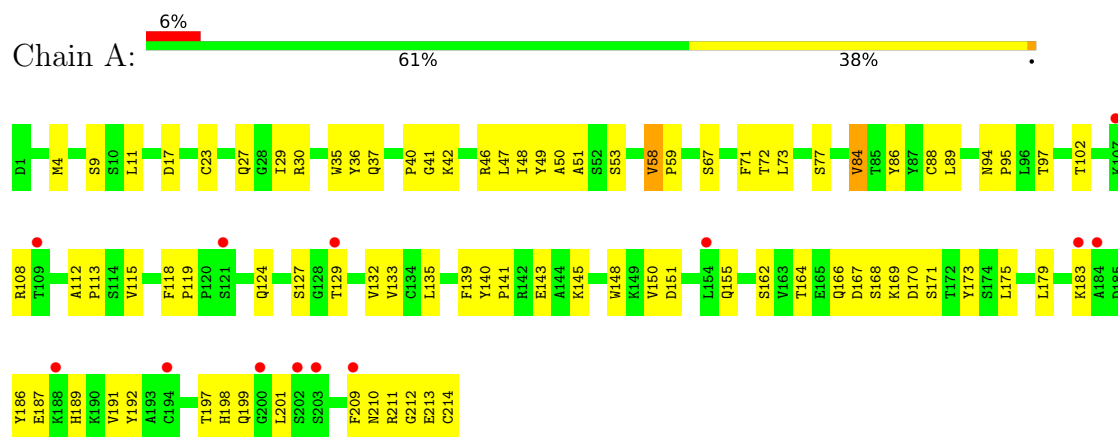
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	19	Total 19	O 19	0	0
4	C	6	Total 6	O 6	0	0
4	D	21	Total 21	O 21	0	0
4	E	37	Total 37	O 37	0	0
4	F	7	Total 7	O 7	0	0

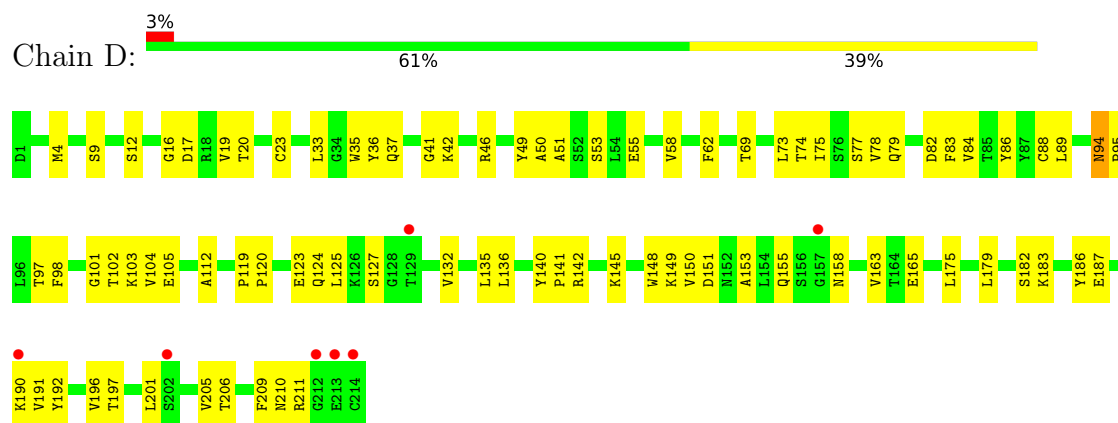
3 Residue-property plots [i](#)

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.

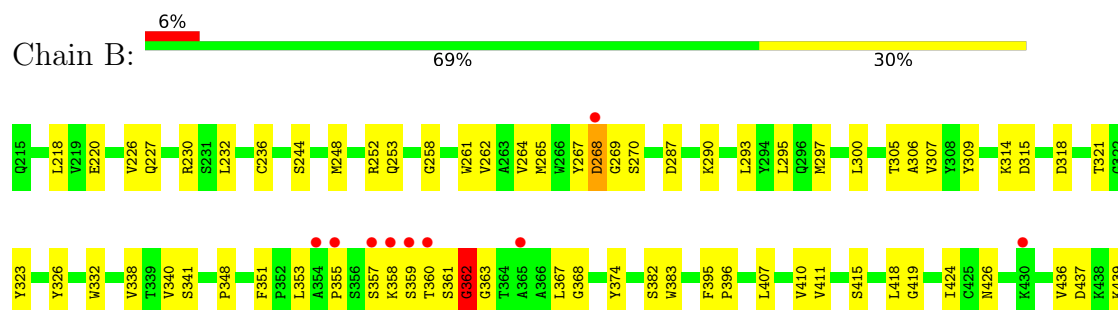
- Molecule 1: Fab heavy chain

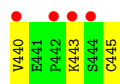


- Molecule 1: Fab heavy chain

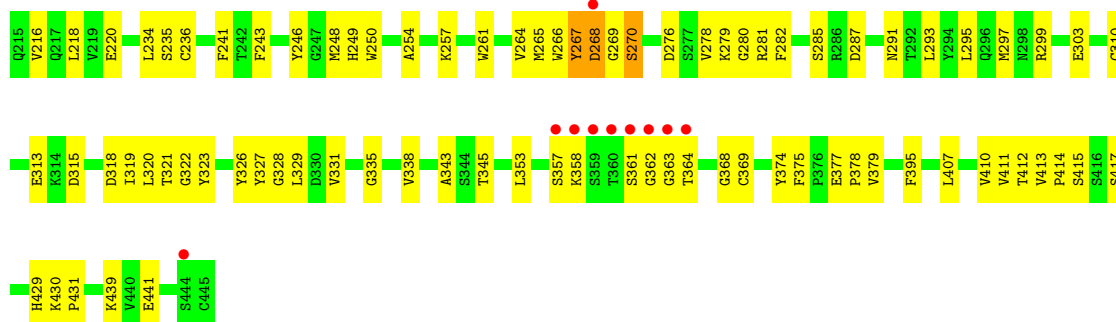


- Molecule 2: Fab light chain

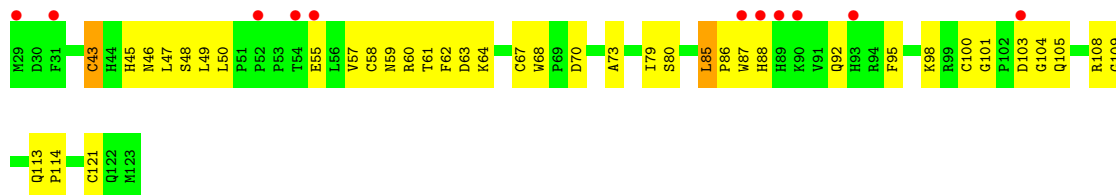




• Molecule 2: Fab light chain



• Molecule 3: Glucagon receptor



• Molecule 3: Glucagon receptor



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.261	Depositor DCC
R_{free} test set	1788 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.65	1/1666 (0.1%)	1.08	6/2259 (0.3%)
1	D	0.63	0/1666	1.08	6/2259 (0.3%)
2	B	0.63	0/1802	1.14	8/2453 (0.3%)
2	E	0.64	0/1800	1.03	6/2450 (0.2%)
3	C	0.63	0/832	1.18	10/1136 (0.9%)
3	F	0.57	0/824	1.05	3/1126 (0.3%)
All	All	0.63	1/8590 (0.0%)	1.09	39/11683 (0.3%)

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 (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	268	ASP	N-CA-C	10.11	123.54	111.82
1	D	95	PRO	N-CA-C	-8.22	95.54	112.47
1	A	94	ASN	C-N-CD	8.15	138.53	120.60
1	A	169	LYS	N-CA-C	7.80	119.56	111.14
3	C	101	GLY	CA-C-N	7.33	127.03	119.56
3	C	101	GLY	C-N-CA	7.33	127.03	119.56
2	E	362	GLY	N-CA-C	7.30	122.19	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	GLY	CA-C-N	7.00	127.16	119.87
3	F	101	GLY	C-N-CA	7.00	127.16	119.87
2	E	270	SER	N-CA-C	-6.98	104.79	113.38
2	B	362	GLY	N-CA-C	6.69	129.03	113.18
2	E	327	TYR	N-CA-C	6.67	121.57	113.17
3	F	102	PRO	N-CA-C	-6.55	105.97	114.03
2	B	419	GLY	N-CA-C	-6.47	105.84	114.25
1	A	212	GLY	N-CA-C	-6.42	106.06	115.63
3	C	104	GLY	N-CA-C	-6.32	106.17	115.72
2	B	436	VAL	N-CA-C	6.01	116.53	108.11
1	D	94	ASN	C-N-CD	-5.97	100.53	125.00
2	B	262	VAL	N-CA-C	5.75	116.17	111.62
1	D	196	VAL	N-CA-C	5.63	115.97	107.75
1	A	115	VAL	N-CA-C	5.62	117.09	108.71
3	C	85	LEU	CA-C-N	5.59	125.42	119.28
3	C	85	LEU	C-N-CA	5.59	125.42	119.28
3	C	109	GLY	CA-C-N	5.59	126.82	119.84
3	C	109	GLY	C-N-CA	5.59	126.82	119.84
3	C	95	PHE	N-CA-C	5.57	117.86	109.23
2	E	267	TYR	N-CA-C	5.56	118.06	111.33
1	D	101	GLY	N-CA-C	5.44	119.53	112.68
1	D	97	THR	N-CA-C	5.41	118.05	109.50
3	C	61	THR	N-CA-C	5.39	116.72	108.42
2	E	361	SER	CB-CA-C	-5.34	110.43	116.63
1	D	69	THR	N-CA-C	5.23	119.82	113.38
2	B	341	SER	N-CA-C	5.20	116.75	108.79
2	E	268	ASP	N-CA-C	5.11	116.70	111.03
1	A	58	VAL	CA-C-N	5.10	126.22	119.84
1	A	58	VAL	C-N-CA	5.10	126.22	119.84
2	B	265	MET	N-CA-C	5.10	117.61	109.81
2	B	262	VAL	N-CA-CB	-5.09	107.46	111.64
3	C	43	CYS	N-CA-C	-5.04	107.30	113.50

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	71	0
1	D	1633	0	1590	55	0
2	B	1758	0	1705	65	0
2	E	1756	0	1700	78	0
3	C	798	0	740	27	0
3	F	790	0	731	35	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	315	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 19.

All (315) 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
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:297:MET:HE1	2:E:338:VAL:HG21	1.53	0.89
1:D:123:GLU:N	1:D:123:GLU:OE1	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:CE1	2:E:248:MET:HE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:243:PHE:HE1	2:E:248:MET:HE2	1.46	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
1:A:41:GLY:C	1:A:42:LYS:HD2	2.15	0.71
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: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
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:D:4:MET:HE3	1:D:23:CYS:SG	2.36	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:254:ALA:HB3	2:E:257:LYS:HG3	1.80	0.64
2:E:318:ASP:CB	2:E:321:THR:HG22	2.27	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
1:A:124:GLN:O	1:A:127:SER:OG	2.16	0.62
2:E:269:GLY:HA3	4:E:501:HOH:O	1.99	0.62
1:D:46:ARG:O	1:D:55:GLU:HG3	2.00	0.62
1:A:46:ARG:HD3	1:A:49:TYR:HB3	1.81	0.62
1:D:191:VAL:HG12	1:D:210:ASN:HB3	1.82	0.62
2:B:270:SER:O	3:C:108:ARG:NH2	2.33	0.61
2:E:234:LEU:HD22	2:E:297:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:268:ASP:CB	2:E:269:GLY:HA2	2.32	0.58
3:F:66:SER:CB	3:F:79:ILE:HD11	2.28	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
2:B:227:GLN:H	2:B:230:ARG:NH1	2.01	0.58
3:F:47:LEU:HD12	3:F:50:LEU:CD1	2.34	0.58
1:D:74:THR:HG23	4:D:302:HOH:O	2.03	0.57
1:A:112:ALA:HB1	1:A:201:LEU:HD12	1.86	0.57
1:A:145:LYS:HB2	1:A:197:THR:HB	1.86	0.57
2:B:355:PRO:HD3	2:B:367:LEU:HB3	1.85	0.57
3:C:63:ASP:HB2	3:C:114:PRO:HB3	1.87	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:4:MET:HE1	1:D:33:LEU:HD12	1.85	0.57
1:D:145:LYS:HD3	1:D:197:THR:HB	1.86	0.57
1:A:191:VAL:HG12	1:A:210:ASN:HB3	1.87	0.57
2:B:230:ARG:HG2	4:B:504:HOH:O	2.03	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:HIS:CE1	3:F:89:HIS:CD2	2.94	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
2:E:357:SER:O	2:E:358:LYS:HB3	2.05	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
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
2:B:267:TYR:OH	2:B:315:ASP:OD1	2.26	0.54
2:B:357:SER:HB2	2:B:358:LYS:C	2.30	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:B:363:GLY:N	2:B:415:SER:HB3	2.23	0.54
1:D:35:TRP:CZ3	1:D:88:CYS:HB3	2.43	0.54
2:E:243:PHE:CD2	2:E:291:ASN:HA	2.43	0.54
2:E:319:ILE:O	4:E:537:HOH:O	2.18	0.54
2:B:362:GLY:HA3	2:B:415:SER:OG	2.06	0.53
1:A:4:MET:HE3	1:A:23:CYS:SG	2.49	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
2:B:232:LEU:HB3	2:B:297:MET:HE3	1.91	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
1:A:164:THR:HG23	2:B:395:PHE:CD1	2.45	0.52
2:E:280:GLY:O	2:E:299:ARG:NH2	2.42	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:A:210:ASN:OD1	1:A:210:ASN:N	2.43	0.51
1:D:151:ASP:OD1	1:D:190:LYS:HB3	2.10	0.51
2:B:297:MET:HE1	2:B:338:VAL:HG21	1.91	0.51
1:A:151:ASP:OD2	1:A:189:HIS:ND1	2.44	0.51
3:F:63:ASP:O	3:F:64:LYS:HB2	2.10	0.51
2:B:382:SER:OG	2:B:426:ASN:HB2	2.10	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:D:175:LEU:HD12	1:D:175:LEU:C	2.36	0.51
2:E:281:ARG:HG2	2:E:299:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HB2	1:A:173:TYR:CE1	2.46	0.50
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
3:F:98:LYS:HD3	3:F:106:TRP:CZ3	2.48	0.49
1:A:199:GLN:C	1:A:201:LEU:H	2.19	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
3:C:73:ALA:HA	3:C:100:CYS:SG	2.53	0.49
2:E:236:CYS:HB3	2:E:293:LEU:HB3	1.94	0.49
2:E:278:VAL:HB	2:E:282:PHE:CG	2.48	0.49
3:C:49:LEU:O	3:C:49:LEU:HD12	2.11	0.49
2:E:220:GLU:CD	4:E:510:HOH:O	2.55	0.49
2:B:287:ASP:OD2	2:B:290:LYS:HE3	2.13	0.49
2:B:360:THR:C	2:B:362:GLY:H	2.21	0.49
2:E:243:PHE:HE1	2:E:248:MET:HE3	1.77	0.49
1:A:49:TYR:O	1:A:53:SER:HB2	2.13	0.48
1:A:113:PRO:HB3	1:A:139:PHE:CD2	2.48	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
1:A:151:ASP:CG	1:A:189:HIS:HD1	2.21	0.48
3:C:45:HIS:O	3:C:48:SER:OG	2.31	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
2:E:343:ALA:HB3	2:E:375:PHE:CZ	2.49	0.48
3:C:49:LEU:C	3:C:50:LEU:HG	2.39	0.47
2:E:243:PHE:CE1	2:E:248:MET:CE	2.83	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
1:A:140:TYR:CG	1:A:141:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:THR:O	2:B:362:GLY:N	2.47	0.47
1:D:186:TYR:CD1	1:D:192:TYR:CZ	3.03	0.47
3:F:113:GLN:O	3:F:113:GLN:HG2	2.14	0.47
1:A:67:SER:HA	1:A:71:PHE:HE1	1.79	0.47
1:A:113:PRO:HB3	1:A:139:PHE:CB	2.39	0.47
1:D:49:TYR:CZ	1:D:53:SER:HB3	2.49	0.47
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
3:C:88:HIS:O	3:C:92:GLN:HB3	2.14	0.46
2:E:268:ASP:HB2	2:E:269:GLY:CA	2.44	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:150:VAL:O	1:D:151:ASP:C	2.56	0.46
1:D:163:VAL:HG22	1:D:175:LEU:HB2	1.97	0.46
1:D:41:GLY:C	1:D:42:LYS:HD2	2.41	0.46
2:E:261:TRP:CZ2	2:E:264:VAL:HG12	2.50	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
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
1:A:48:ILE:HG23	1:A:53:SER:O	2.16	0.45
2:B:332:TRP:CD1	2:B:332:TRP:N	2.83	0.45
1:D:175:LEU:HA	2:E:395:PHE:HE2	1.81	0.45
1:D:145:LYS:HD2	1:D:145:LYS:H	1.81	0.45
2:B:268:ASP:N	2:B:269:GLY:HA2	2.32	0.45
2:B:439:LYS:HG3	2:B:440:VAL:N	2.31	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
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
3:F:98:LYS:HB3	3:F:106:TRP:CZ3	2.52	0.45
1:A:175:LEU:C	1:A:175:LEU:HD12	2.42	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
2:B:295:LEU:HD12	2:B:295:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:35:LYS:HD2	3:F:83:TRP:HZ3	1.82	0.45
3:F:88:HIS:HE1	3:F:89:HIS:HD2	1.64	0.45
1:A:199:GLN:C	1:A:201:LEU:N	2.73	0.44
2:B:407:LEU:HD12	2:B:407:LEU:C	2.42	0.44
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:320:LEU:HD21	3:F:32:LEU:HD21	1.99	0.44
2:E:430:LYS:N	2:E:431:PRO:HD3	2.31	0.44
3:C:60:ARG:HB3	3:C:70:ASP:OD1	2.17	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
1:D:124:GLN:O	1:D:127:SER:OG	2.34	0.44
2:E:281:ARG:HG2	2:E:299:ARG:NH2	2.32	0.44
1:A:108:ARG:HD2	1:A:170:ASP:O	2.18	0.44
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.78	0.44
2:B:363:GLY:O	2:B:415:SER:N	2.46	0.44
1:D:135:LEU:CD2	2:E:410:VAL:HG11	2.47	0.44
3:F:103:ASP:OD2	3:F:105:GLN:HB2	2.17	0.44
1:A:124:GLN:HG3	2:B:351:PHE:CE2	2.52	0.43
3:C:87:TRP:NE1	3:C:121:CYS:O	2.44	0.43
2:E:377:GLU:HB3	2:E:378:PRO:HA	2.00	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
3:F:45:HIS:O	3:F:46:ASN:C	2.60	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
1:A:72:THR:HG22	4:A:306:HOH:O	2.18	0.43
2:B:314:LYS:HG3	2:B:315:ASP:N	2.32	0.43
1:A:143:GLU:CD	1:A:143:GLU:H	2.24	0.43
2:E:353:LEU:HD12	2:E:368:GLY:C	2.44	0.43
2:E:218:LEU:HD23	2:E:218:LEU:HA	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
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
3:C:68:TRP:CE2	3:C:98:LYS:HD2	2.53	0.42
2:E:353:LEU:HD12	2:E:369:CYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:58:CYS:O	3:C:59:ASN:C	2.60	0.42
2:E:234:LEU:CD2	2:E:297:MET:HE2	2.48	0.42
2:E:287:ASP:OD1	2:E:287:ASP:C	2.63	0.42
2:E:407:LEU:HD12	2:E:407:LEU:C	2.45	0.42
1:D:19:VAL:HG23	1:D:78:VAL:HG22	2.01	0.42
2:E:265:MET:HE3	2:E:265:MET:HB2	1.94	0.42
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:210:ASN:OD1	1:D:210:ASN:N	2.53	0.42
2:E:265:MET:HE2	2:E:266:TRP:O	2.20	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:C:85:LEU:HA	3:C:86:PRO:HD3	1.85	0.42
2:E:343:ALA:HB3	2:E:375:PHE:CE2	2.55	0.42
3:F:47:LEU:HG	3:F:60:ARG:HD3	2.01	0.42
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
3:F:37:LYS:O	3:F:38:LEU:C	2.62	0.41
2:B:252:ARG:HA	2:B:307:VAL:O	2.20	0.41
2:E:439:LYS:HD3	2:E:441:GLU:CG	2.50	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
2:B:220:GLU:OE1	2:B:309:TYR:HA	2.21	0.41
1:D:182:SER:O	1:D:183:LYS:C	2.63	0.41
1:A:17:ASP:O	1:A:77:SER:HA	2.20	0.41
1:D:55:GLU:OE2	1:D:55:GLU:HA	2.19	0.41
3:C:55:GLU:O	3:C:57:VAL:HG13	2.20	0.41
1:D:142:ARG:HH11	1:D:163:VAL:CG1	2.34	0.41
2:B:348:PRO:HB3	2:B:374:TYR:HB3	2.02	0.41
2:E:249:HIS:O	2:E:310:CYS:HA	2.21	0.41
1:A:27:GLN:O	1:A:29:ILE:HG23	2.21	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
2:B:261:TRP:HZ2	2:B:264:VAL:CG1	2.34	0.41
1:D:20:THR:OG1	1:D:74:THR:HG22	2.20	0.41
1:D:62:PHE:CE1	1:D:75:ILE:HD13	2.56	0.41
1:A:30:ARG:HD2	4:A:310:HOH:O	2.20	0.41
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:O	1:A:86:TYR:HA	2.21	0.40
2:B:305:THR:O	2:B:306:ALA:HB2	2.20	0.40
1:D:148:TRP:HB2	1:D:155:GLN:HB2	2.03	0.40
1:A:11:LEU:C	1:A:11:LEU:HD12	2.46	0.40
1:A:198:HIS:CG	1:A:199:GLN:N	2.90	0.40
2:E:267:TYR:OH	2:E:315:ASP:OD1	2.34	0.40
3:F:105:GLN:HA	4:F:206:HOH:O	2.21	0.40
2:B:244:SER:O	2:B:267:TYR:CD1	2.74	0.40
1:D:136:LEU:N	1:D:136:LEU:HD12	2.36	0.40
2:E:216:VAL:HG12	2:E:331:VAL:HG21	2.03	0.40
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%)	24	40
1	D	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	24	40
2	B	229/231 (99%)	215 (94%)	12 (5%)	2 (1%)	14	26
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%)	30	47

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	214/214 (100%)	0.59	13 (6%)	27 26	23, 59, 119, 149	0
1	D	214/214 (100%)	-0.01	7 (3%)	49 47	9, 44, 85, 123	0
2	B	231/231 (100%)	0.23	13 (5%)	30 29	18, 45, 95, 147	0
2	E	231/231 (100%)	-0.13	10 (4%)	40 38	14, 36, 82, 141	0
3	C	95/95 (100%)	0.70	11 (11%)	9 9	28, 60, 113, 147	0
3	F	94/95 (98%)	0.17	3 (3%)	50 48	20, 49, 90, 112	0
All	All	1079/1080 (99%)	0.21	57 (5%)	32 31	9, 46, 105, 149	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	358	LYS	7.1
2	E	358	LYS	6.1
2	E	362	GLY	5.0
1	D	212	GLY	4.7
2	E	360	THR	4.3
3	C	31	PHE	4.3
2	E	359	SER	4.2
1	A	188	LYS	3.9
2	B	268	ASP	3.6
2	B	359	SER	3.6
2	E	357	SER	3.3
2	B	444	SER	3.2
3	C	89	HIS	3.1
1	A	184	ALA	3.1
2	E	363	GLY	3.1
2	E	361	SER	3.0
2	E	268	ASP	2.9
1	D	214	CYS	2.9
1	A	154	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	31	PHE	2.8
2	B	354	ALA	2.8
2	B	360	THR	2.7
1	A	109	THR	2.7
1	D	190	LYS	2.7
3	C	93	HIS	2.6
3	C	55	GLU	2.6
3	C	103	ASP	2.6
3	C	29	MET	2.5
2	B	365	ALA	2.4
1	D	202	SER	2.4
2	B	357	SER	2.4
3	C	87	TRP	2.4
1	A	209	PHE	2.3
2	E	364	THR	2.3
3	F	30	ASP	2.3
2	B	440	VAL	2.3
3	C	88	HIS	2.2
1	A	202	SER	2.2
2	B	430	LYS	2.2
2	B	355	PRO	2.2
2	B	443	LYS	2.2
1	A	200	GLY	2.1
1	A	121	SER	2.1
1	D	213	GLU	2.1
1	D	129	THR	2.1
3	C	54	THR	2.1
1	A	107	LYS	2.1
3	C	52	PRO	2.1
1	A	203	SER	2.1
2	E	444	SER	2.1
2	B	442	PRO	2.0
1	D	157	GLY	2.0
1	A	194	CYS	2.0
1	A	183	LYS	2.0
3	C	90	LYS	2.0
1	A	129	THR	2.0
3	F	89	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.