



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:55 AM GMT

PDB ID : 1D00
Title : STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 IN COM-
PLEX WITH A 5-RESIDUE CD40 PEPTIDE
Authors : Ye, H.; Park, Y.C.; Kreishman, M.; Kieff, E.; Wu, H.
Deposited on : 1999-09-07
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

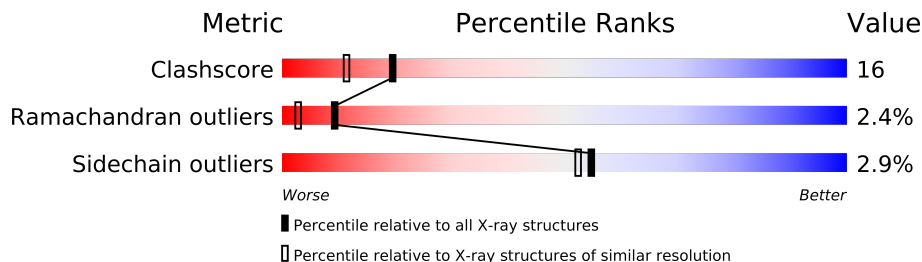
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	
1	B	168	
1	C	168	
1	D	168	
1	E	168	
1	F	168	
1	G	168	
1	H	168	
2	I	7	
2	J	7	
2	K	7	
2	L	7	
2	M	7	
2	N	7	
2	O	7	
2	P	7	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10670 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	B	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	C	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	D	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	E	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	F	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	G	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	H	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	PRO	CONFLICT	GB 1363002
A	365	ARG	LEU	CONFLICT	GB 1363002
B	362	ALA	PRO	CONFLICT	GB 1363002
B	365	ARG	LEU	CONFLICT	GB 1363002
C	362	ALA	PRO	CONFLICT	GB 1363002
C	365	ARG	LEU	CONFLICT	GB 1363002
D	362	ALA	PRO	CONFLICT	GB 1363002
D	365	ARG	LEU	CONFLICT	GB 1363002
E	362	ALA	PRO	CONFLICT	GB 1363002
E	365	ARG	LEU	CONFLICT	GB 1363002
F	362	ALA	PRO	CONFLICT	GB 1363002
F	365	ARG	LEU	CONFLICT	GB 1363002

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	362	ALA	PRO	CONFLICT	GB 1363002
G	365	ARG	LEU	CONFLICT	GB 1363002
H	362	ALA	PRO	CONFLICT	GB 1363002
H	365	ARG	LEU	CONFLICT	GB 1363002

- Molecule 2 is a protein called B-CELL SURFACE ANTIGEN CD40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	J	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	K	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	L	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	M	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	N	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	O	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	P	7	Total	C	N	O	0	0	1
			43	26	7	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	3	Total	O	0	0
			3	3		
3	C	11	Total	O	0	0
			11	11		
3	D	7	Total	O	0	0
			7	7		
3	E	5	Total	O	0	0
			5	5		
3	F	9	Total	O	0	0
			9	9		
3	G	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	13	Total 13	O 13	0	0
3	K	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0

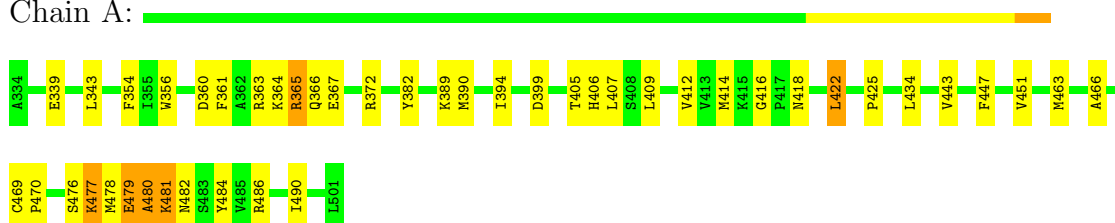
3 Residue-property plots

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.

Note EDS was not executed.

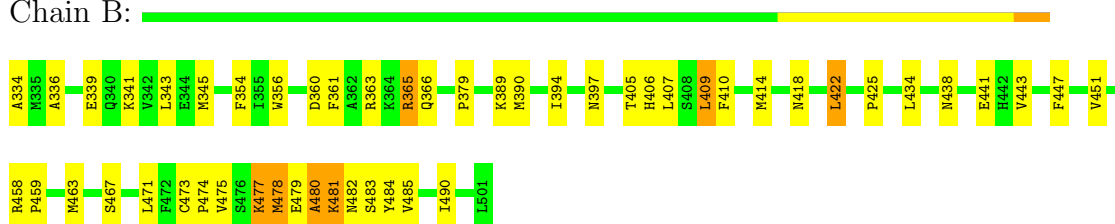
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain A:



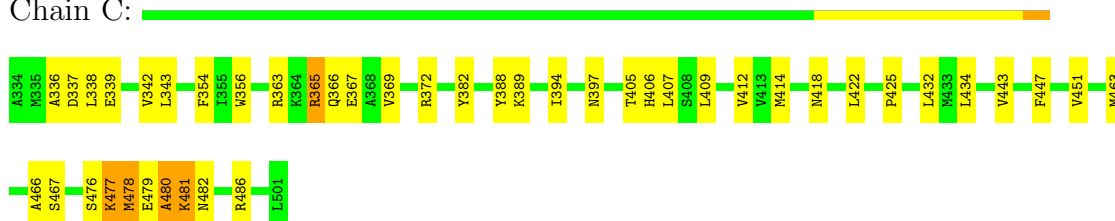
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain B:



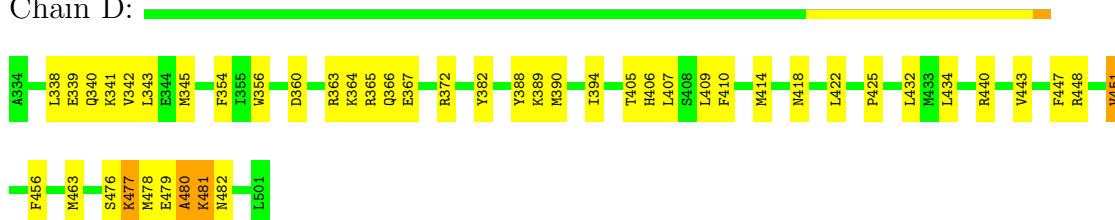
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain C:



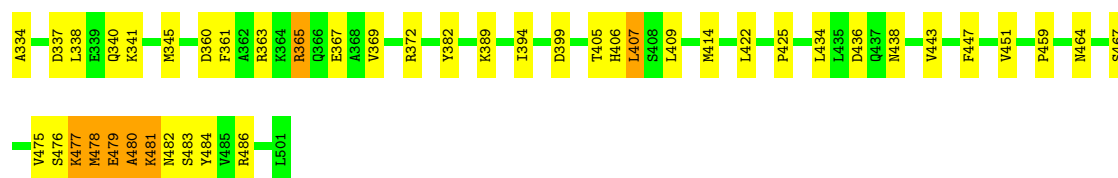
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain D:



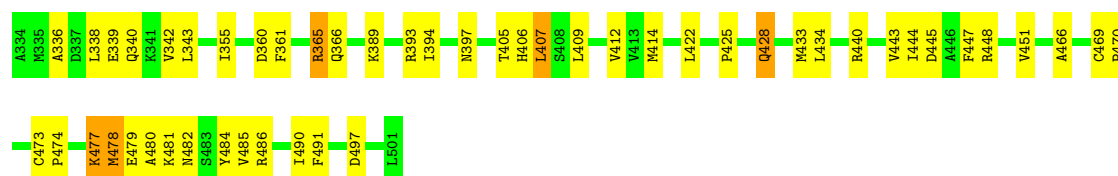
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain E: 



- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain F: 



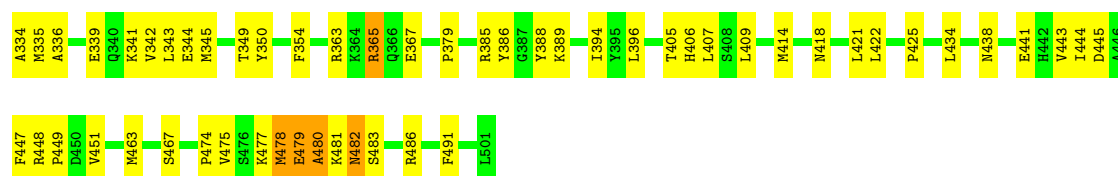
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain G: 



- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain H: 



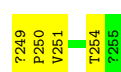
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain I: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain J: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain K: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain L: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain M: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain N: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain O: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain P: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	111.40Å 111.40Å 111.40Å 103.70° 103.70° 103.70°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10670	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	0.44	0/1312	0.71	0/1781
1	B	0.42	0/1312	0.71	0/1781
1	C	0.43	0/1312	0.72	0/1781
1	D	0.44	0/1312	0.71	0/1781
1	E	0.43	0/1312	0.70	1/1781 (0.1%)
1	F	0.44	0/1312	0.73	1/1781 (0.1%)
1	G	0.42	0/1312	0.71	0/1781
1	H	0.41	0/1312	0.71	0/1781
2	I	0.42	0/40	0.74	0/55
2	J	0.51	0/40	0.77	0/55
2	K	0.47	0/40	0.69	0/55
2	L	0.48	0/40	0.81	0/55
2	M	0.44	0/40	0.73	0/55
2	N	0.47	0/40	0.73	0/55
2	O	0.49	0/40	0.71	0/55
2	P	0.50	0/40	0.79	0/55
All	All	0.43	0/10816	0.71	2/14688 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	407	LEU	N-CA-C	-5.20	96.96	111.00
1	F	407	LEU	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1282	0	1242	36	0
1	B	1282	0	1242	45	0
1	C	1282	0	1242	37	0
1	D	1282	0	1242	43	0
1	E	1282	0	1242	41	0
1	F	1282	0	1242	43	0
1	G	1282	0	1242	44	0
1	H	1282	0	1242	53	0
2	I	43	0	40	3	0
2	J	43	0	40	7	0
2	K	43	0	40	6	0
2	L	43	0	40	1	0
2	M	43	0	40	3	0
2	N	43	0	40	1	0
2	O	43	0	40	4	0
2	P	43	0	40	9	0
3	A	12	0	0	1	0
3	B	3	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	3	0
3	E	5	0	0	1	0
3	F	9	0	0	4	0
3	G	8	0	0	0	0
3	H	13	0	0	5	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	10670	0	10256	337	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (337) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:425:PRO:HG3	1:H:451:VAL:HG13	1.41	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:PRO:HG3	1:A:451:VAL:HG13	1.43	0.99
1:H:394:ILE:HD11	1:H:407:LEU:HD21	1.41	0.99
1:G:389:LYS:HG2	1:G:414:MET:HE3	1.46	0.95
1:E:425:PRO:HG3	1:E:451:VAL:HG13	1.51	0.93
3:F:1052:HOH:O	1:H:421:LEU:HD21	1.69	0.92
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.52	0.88
1:A:447:PHE:CD1	2:I:250:PRO:HG3	2.09	0.87
1:F:339:GLU:O	1:F:343:LEU:HD13	1.73	0.87
1:F:394:ILE:HD11	1:F:407:LEU:HD21	1.56	0.86
1:C:447:PHE:CD1	2:K:250:PRO:HG3	2.10	0.86
1:D:425:PRO:HB2	3:D:1021:HOH:O	1.77	0.85
1:F:428:GLN:HG3	1:F:497:ASP:O	1.78	0.84
1:D:409:LEU:HD22	1:D:432:LEU:HD13	1.57	0.84
1:H:447:PHE:CD1	2:P:250:PRO:HG3	2.11	0.84
1:D:447:PHE:CD1	2:L:250:PRO:HG3	2.14	0.82
1:A:425:PRO:CG	1:A:451:VAL:HG13	2.10	0.81
1:B:425:PRO:HG3	1:B:451:VAL:HG13	1.60	0.81
1:H:451:VAL:HA	3:H:1032:HOH:O	1.78	0.81
1:E:367:GLU:HG2	1:E:372:ARG:NH2	1.96	0.81
1:G:389:LYS:HG2	1:G:414:MET:CE	2.11	0.80
1:E:394:ILE:HD11	1:E:407:LEU:HD21	1.64	0.80
1:F:447:PHE:CD1	2:N:250:PRO:HG3	2.17	0.80
2:J:254:THR:O	2:J:254:THR:HG22	1.81	0.80
1:E:447:PHE:CD1	2:M:250:PRO:HG3	2.18	0.79
1:F:389:LYS:HG2	1:F:414:MET:HE3	1.65	0.79
1:C:434:LEU:HB3	1:C:443:VAL:HB	1.63	0.78
1:H:389:LYS:HG2	1:H:414:MET:HE3	1.67	0.77
1:C:389:LYS:HG2	1:C:414:MET:HE3	1.66	0.77
1:A:394:ILE:HD11	1:A:407:LEU:HD21	1.66	0.76
1:A:389:LYS:HG2	1:A:414:MET:HE3	1.67	0.75
1:C:339:GLU:O	1:C:343:LEU:HD13	1.86	0.75
1:E:425:PRO:CG	1:E:451:VAL:HG13	2.17	0.73
1:E:389:LYS:HG2	1:E:414:MET:HE3	1.69	0.72
1:G:447:PHE:CD1	2:O:250:PRO:HG3	2.24	0.72
1:H:425:PRO:CG	1:H:451:VAL:HG13	2.19	0.72
1:F:425:PRO:HG3	1:F:451:VAL:HG13	1.70	0.72
1:B:447:PHE:CD1	2:J:250:PRO:HG3	2.25	0.71
1:A:434:LEU:HB3	1:A:443:VAL:HB	1.69	0.71
1:A:425:PRO:HG3	1:A:451:VAL:CG1	2.19	0.71
1:F:389:LYS:HG2	1:F:414:MET:CE	2.20	0.71
1:H:481:LYS:O	1:H:482:ASN:HB2	1.91	0.71
1:H:394:ILE:CD1	1:H:407:LEU:HD21	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:GLU:O	1:A:343:LEU:HD13	1.91	0.71
1:H:434:LEU:HB3	1:H:443:VAL:HB	1.73	0.71
1:D:389:LYS:HG2	1:D:414:MET:CE	2.20	0.70
1:F:448:ARG:HG3	2:J:249:ACE:H1	1.72	0.70
1:D:448:ARG:NH2	2:P:251:VAL:HG22	2.06	0.70
1:H:478:MET:SD	1:H:479:GLU:N	2.65	0.70
1:G:365:ARG:O	1:G:369:VAL:HG23	1.92	0.69
1:D:456:PHE:HB2	3:D:1021:HOH:O	1.92	0.69
1:G:481:LYS:O	1:G:482:ASN:HB2	1.92	0.69
1:A:478:MET:HE1	1:A:490:ILE:HG21	1.75	0.68
1:F:434:LEU:HB3	1:F:443:VAL:HB	1.73	0.68
1:A:389:LYS:HG2	1:A:414:MET:CE	2.23	0.68
2:K:254:THR:HG22	2:K:254:THR:O	1.92	0.68
1:G:434:LEU:HB3	1:G:443:VAL:HB	1.75	0.67
1:E:367:GLU:HG2	1:E:372:ARG:HH21	1.60	0.67
1:C:480:ALA:O	1:C:481:LYS:O	2.14	0.67
1:H:334:ALA:O	1:H:336:ALA:N	2.24	0.66
1:D:363:ARG:NH1	1:D:367:GLU:OE1	2.28	0.66
1:A:405:THR:OG1	1:A:406:HIS:HD2	1.80	0.66
1:C:409:LEU:HD22	1:C:432:LEU:HD13	1.77	0.65
1:G:418:ASN:O	1:G:422:LEU:HD13	1.95	0.65
1:G:394:ILE:HD11	1:G:407:LEU:HD21	1.77	0.65
1:D:448:ARG:HG3	2:P:249:ACE:H1	1.77	0.65
1:B:434:LEU:HB3	1:B:443:VAL:HB	1.78	0.65
1:D:363:ARG:HG2	1:D:363:ARG:HH11	1.63	0.64
1:E:478:MET:SD	1:E:479:GLU:N	2.71	0.64
1:E:478:MET:HB3	1:E:484:TYR:CD1	2.33	0.64
1:C:363:ARG:HG2	1:C:363:ARG:HH11	1.63	0.64
1:A:486:ARG:HG3	1:A:486:ARG:HH11	1.63	0.63
1:B:389:LYS:HG2	1:B:414:MET:HE3	1.80	0.63
1:C:418:ASN:O	1:C:422:LEU:HD13	1.98	0.63
1:D:338:LEU:O	1:D:342:VAL:HG23	1.98	0.63
1:G:478:MET:O	1:G:480:ALA:N	2.30	0.63
1:C:389:LYS:HG2	1:C:414:MET:CE	2.29	0.62
1:F:433:MET:CE	1:F:444:ILE:HD12	2.29	0.62
1:H:425:PRO:HG3	1:H:451:VAL:CG1	2.23	0.62
1:H:389:LYS:HG2	1:H:414:MET:CE	2.29	0.62
1:F:365:ARG:NH2	1:F:397:ASN:OD1	2.33	0.62
1:G:385:ARG:HG2	1:H:349:THR:HG22	1.82	0.61
1:H:341:LYS:O	1:H:345:MET:HG3	2.00	0.61
1:A:418:ASN:O	1:A:422:LEU:HD13	2.01	0.61
1:C:478:MET:SD	1:C:479:GLU:N	2.74	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:342:VAL:HG13	1:E:345:MET:SD	2.41	0.61
1:F:478:MET:SD	1:F:479:GLU:N	2.73	0.61
1:E:341:LYS:O	1:E:345:MET:HG3	2.01	0.60
1:C:394:ILE:HD11	1:C:407:LEU:HD21	1.82	0.60
1:B:394:ILE:HD11	1:B:407:LEU:HD21	1.83	0.60
1:H:481:LYS:O	1:H:482:ASN:CB	2.49	0.59
1:E:434:LEU:HB3	1:E:443:VAL:HB	1.83	0.59
1:B:405:THR:O	1:B:475:VAL:HG23	2.02	0.59
1:H:389:LYS:HE2	1:H:414:MET:HE3	1.83	0.59
1:G:409:LEU:HD22	1:G:432:LEU:HD13	1.83	0.59
1:B:405:THR:C	1:B:475:VAL:HG23	2.22	0.59
1:C:414:MET:HG2	1:C:463:MET:HG2	1.85	0.59
1:E:360:ASP:OD1	1:E:363:ARG:NE	2.28	0.59
1:H:365:ARG:HG2	3:H:1001:HOH:O	2.03	0.58
1:A:394:ILE:CD1	1:A:407:LEU:HD21	2.32	0.58
1:F:491:PHE:HB2	3:F:1052:HOH:O	2.03	0.58
1:B:485:VAL:HG22	1:B:490:ILE:CG2	2.32	0.58
1:D:405:THR:OG1	1:D:406:HIS:HD2	1.87	0.58
1:H:486:ARG:HG3	1:H:486:ARG:HH11	1.68	0.58
1:D:434:LEU:HB3	1:D:443:VAL:HB	1.86	0.58
1:G:361:PHE:O	1:G:365:ARG:HB2	2.03	0.57
1:B:467:SER:OG	2:J:250:PRO:HB2	2.04	0.57
1:H:363:ARG:O	1:H:367:GLU:HG3	2.05	0.57
1:F:433:MET:HE3	1:F:444:ILE:HD12	1.86	0.57
1:B:354:PHE:CE2	1:B:356:TRP:HB2	2.40	0.57
1:E:478:MET:O	1:E:480:ALA:N	2.37	0.56
1:F:338:LEU:O	1:F:342:VAL:HG23	2.05	0.56
1:F:394:ILE:CD1	1:F:407:LEU:HD21	2.31	0.56
1:F:412:VAL:HG22	1:F:466:ALA:HB2	1.87	0.56
1:A:360:ASP:OD1	1:A:363:ARG:NE	2.33	0.56
1:D:367:GLU:HG2	1:D:372:ARG:HH21	1.71	0.56
1:B:425:PRO:CG	1:B:451:VAL:HG13	2.35	0.56
1:H:438:ASN:ND2	1:H:483:SER:HB3	2.20	0.56
1:F:389:LYS:HE2	1:F:414:MET:HE3	1.86	0.56
1:B:478:MET:HB3	1:B:484:TYR:CD1	2.41	0.56
1:E:337:ASP:O	1:E:340:GLN:N	2.30	0.55
1:E:405:THR:OG1	1:E:406:HIS:HD2	1.89	0.55
1:B:334:ALA:C	1:B:336:ALA:N	2.59	0.55
1:D:448:ARG:HH21	2:P:251:VAL:HG22	1.71	0.55
1:G:481:LYS:O	1:G:482:ASN:CB	2.53	0.55
1:H:451:VAL:HG12	1:H:451:VAL:O	2.06	0.55
2:J:254:THR:O	2:J:254:THR:CG2	2.53	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:334:ALA:C	1:H:336:ALA:H	2.09	0.55
1:G:405:THR:O	1:G:475:VAL:HG23	2.07	0.55
1:C:365:ARG:HH21	1:C:397:ASN:HA	1.72	0.55
1:G:425:PRO:HG2	1:G:451:VAL:HG12	1.89	0.55
1:C:481:LYS:O	1:C:482:ASN:HB2	2.06	0.54
1:F:425:PRO:CG	1:F:451:VAL:HG13	2.36	0.54
1:D:367:GLU:HG2	1:D:372:ARG:NH2	2.23	0.54
1:B:478:MET:SD	1:B:479:GLU:N	2.80	0.54
1:H:418:ASN:O	1:H:422:LEU:HD13	2.07	0.54
1:B:481:LYS:O	1:B:482:ASN:HB2	2.06	0.54
1:G:389:LYS:HE2	1:G:414:MET:HE3	1.90	0.54
1:H:396:LEU:HD22	3:H:1001:HOH:O	2.07	0.54
1:G:360:ASP:HB2	1:G:364:LYS:HE3	1.89	0.54
1:E:486:ARG:HH11	1:E:486:ARG:HG3	1.73	0.54
1:G:425:PRO:CG	1:G:451:VAL:HG12	2.38	0.53
1:G:412:VAL:HG22	1:G:466:ALA:HB2	1.89	0.53
1:A:478:MET:SD	1:A:479:GLU:N	2.81	0.53
1:F:434:LEU:HD21	1:F:478:MET:HG2	1.90	0.53
1:E:389:LYS:HG2	1:E:414:MET:CE	2.36	0.53
1:E:425:PRO:HG3	1:E:451:VAL:CG1	2.33	0.53
1:E:451:VAL:HG12	1:E:451:VAL:O	2.09	0.53
1:E:467:SER:OG	2:M:250:PRO:HB2	2.09	0.53
1:E:334:ALA:HB2	3:E:1061:HOH:O	2.09	0.53
1:G:390:MET:O	1:G:414:MET:HE1	2.09	0.53
1:E:405:THR:O	1:E:475:VAL:HG23	2.08	0.53
1:D:418:ASN:O	1:D:422:LEU:HD13	2.09	0.53
1:H:339:GLU:O	1:H:343:LEU:HD13	2.09	0.53
1:G:354:PHE:HZ	1:G:379:PRO:HD2	1.72	0.53
1:A:481:LYS:O	1:A:482:ASN:HB2	2.09	0.52
1:G:389:LYS:CG	1:G:414:MET:HE3	2.29	0.52
1:E:365:ARG:O	1:E:369:VAL:HG23	2.09	0.52
1:B:441:GLU:HA	1:F:440:ARG:HA	1.91	0.52
1:A:478:MET:HB2	1:A:484:TYR:HB2	1.90	0.52
1:A:479:GLU:O	1:A:480:ALA:O	2.28	0.52
1:C:476:SER:O	1:C:477:LYS:O	2.27	0.51
1:F:393:ARG:NH1	3:F:1012:HOH:O	2.43	0.51
1:E:394:ILE:CD1	1:E:407:LEU:HD21	2.38	0.51
1:D:448:ARG:HG3	2:P:249:ACE:CH3	2.39	0.51
1:G:478:MET:HB3	1:G:484:TYR:CD1	2.46	0.51
1:G:409:LEU:HD23	1:G:410:PHE:N	2.26	0.51
1:E:478:MET:HB2	1:E:484:TYR:HB2	1.93	0.51
1:B:414:MET:HG2	1:B:463:MET:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:ARG:HH21	1:B:397:ASN:HA	1.76	0.51
1:D:409:LEU:HD23	1:D:410:PHE:N	2.26	0.51
1:H:478:MET:O	1:H:480:ALA:N	2.44	0.51
1:H:354:PHE:HZ	1:H:379:PRO:HD2	1.75	0.51
1:G:467:SER:OG	2:O:250:PRO:HB2	2.11	0.51
1:F:405:THR:OG1	1:F:406:HIS:HD2	1.93	0.50
1:B:354:PHE:HZ	1:B:379:PRO:HD2	1.76	0.50
1:D:480:ALA:O	1:D:481:LYS:O	2.30	0.50
1:A:367:GLU:HG2	1:A:372:ARG:HH21	1.76	0.50
1:D:389:LYS:CG	1:D:414:MET:HE3	2.34	0.50
1:F:478:MET:HB2	1:F:484:TYR:HB2	1.92	0.50
1:E:477:LYS:O	1:E:478:MET:O	2.29	0.50
1:C:365:ARG:O	1:C:369:VAL:HG23	2.12	0.50
1:D:394:ILE:HD11	1:D:407:LEU:HD21	1.93	0.50
1:H:405:THR:O	1:H:475:VAL:HG23	2.13	0.49
1:H:388:TYR:CD2	1:H:422:LEU:HD23	2.48	0.49
1:B:478:MET:O	1:B:479:GLU:CB	2.60	0.49
1:D:360:ASP:HB3	1:D:364:LYS:HE3	1.93	0.49
1:H:451:VAL:CG1	1:H:451:VAL:O	2.61	0.49
1:D:477:LYS:O	1:D:482:ASN:OD1	2.32	0.48
1:H:467:SER:OG	2:P:250:PRO:HB2	2.13	0.48
1:G:478:MET:HE2	1:G:485:VAL:HG23	1.95	0.48
1:B:334:ALA:C	1:B:336:ALA:H	2.16	0.48
1:H:444:ILE:HG12	1:H:445:ASP:N	2.27	0.48
1:D:388:TYR:CD2	1:D:422:LEU:HD23	2.48	0.48
1:A:354:PHE:CE2	1:A:356:TRP:HB2	2.49	0.48
1:B:485:VAL:HG22	1:B:490:ILE:HG22	1.95	0.48
1:C:338:LEU:HG	1:E:338:LEU:HD21	1.94	0.48
1:A:389:LYS:HE2	1:A:414:MET:HE3	1.95	0.48
1:F:486:ARG:HH11	1:F:486:ARG:HG3	1.79	0.48
1:H:447:PHE:CG	2:P:250:PRO:HG3	2.49	0.48
1:C:363:ARG:HG2	1:C:363:ARG:NH1	2.28	0.48
1:A:416:GLY:HA3	3:A:1067:HOH:O	2.13	0.48
1:G:363:ARG:O	1:G:367:GLU:HG3	2.14	0.48
1:F:338:LEU:HD11	1:G:342:VAL:HG21	1.96	0.48
1:A:476:SER:O	1:A:477:LYS:C	2.52	0.48
1:D:390:MET:O	1:D:414:MET:HE1	2.14	0.48
1:F:448:ARG:HG3	2:J:249:ACE:CH3	2.43	0.48
1:B:343:LEU:HD12	1:B:343:LEU:N	2.29	0.47
1:B:389:LYS:C	1:B:390:MET:HG3	2.33	0.47
1:G:385:ARG:HH11	1:G:385:ARG:HG3	1.78	0.47
1:D:414:MET:HG2	1:D:463:MET:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:MET:HG2	1:A:463:MET:HG2	1.95	0.47
1:D:476:SER:O	1:D:477:LYS:C	2.52	0.47
1:B:477:LYS:C	1:B:478:MET:O	2.50	0.47
1:B:405:THR:OG1	1:B:406:HIS:HD2	1.97	0.47
1:H:396:LEU:HB3	3:H:1001:HOH:O	2.15	0.47
1:B:339:GLU:O	1:B:343:LEU:CD1	2.63	0.47
1:D:382:TYR:CD1	1:D:382:TYR:N	2.82	0.47
1:D:478:MET:SD	1:D:479:GLU:N	2.87	0.47
1:C:447:PHE:CG	2:K:250:PRO:HG3	2.50	0.47
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.80	0.47
1:B:479:GLU:O	1:B:480:ALA:O	2.33	0.47
1:C:365:ARG:NH2	1:C:397:ASN:OD1	2.48	0.47
1:A:382:TYR:CD1	1:A:382:TYR:N	2.82	0.47
1:D:448:ARG:HH21	2:P:251:VAL:CG2	2.29	0.46
1:G:478:MET:C	1:G:480:ALA:H	2.18	0.46
1:C:405:THR:OG1	1:C:406:HIS:HD2	1.99	0.46
1:E:438:ASN:ND2	1:E:483:SER:CB	2.77	0.46
1:E:407:LEU:C	1:E:407:LEU:HD23	2.35	0.46
1:E:438:ASN:ND2	1:E:483:SER:HB3	2.31	0.46
1:F:355:ILE:HD12	1:H:386:TYR:CG	2.51	0.46
1:C:367:GLU:HG2	1:C:372:ARG:NH2	2.31	0.46
1:H:480:ALA:C	1:H:481:LYS:O	2.53	0.46
1:G:385:ARG:NH1	1:G:385:ARG:HG3	2.31	0.46
1:E:382:TYR:CD1	1:E:382:TYR:N	2.84	0.46
1:C:425:PRO:HG3	1:C:451:VAL:HG13	1.97	0.46
1:C:339:GLU:O	1:C:343:LEU:CD1	2.61	0.46
1:C:336:ALA:C	1:C:338:LEU:H	2.20	0.46
1:B:409:LEU:HD23	1:B:410:PHE:N	2.31	0.46
1:G:399:ASP:OD1	2:O:254:THR:HB	2.17	0.45
1:H:344:GLU:O	1:H:345:MET:C	2.54	0.45
1:H:422:LEU:CD1	1:H:422:LEU:N	2.79	0.45
1:F:448:ARG:NH2	2:J:251:VAL:HG22	2.31	0.45
2:K:254:THR:CG2	2:K:254:THR:O	2.62	0.45
1:B:478:MET:CB	1:B:484:TYR:CD1	3.00	0.45
1:C:354:PHE:CE2	1:C:356:TRP:HB2	2.52	0.45
1:G:339:GLU:O	1:G:340:GLN:C	2.54	0.45
1:F:478:MET:HB3	1:F:484:TYR:CD1	2.52	0.44
1:G:434:LEU:HD21	1:G:478:MET:HE3	1.98	0.44
1:A:360:ASP:HB3	1:A:364:LYS:HE3	2.00	0.44
1:B:478:MET:HE2	1:B:485:VAL:HG23	1.98	0.44
1:F:444:ILE:CG1	1:F:445:ASP:N	2.81	0.44
1:F:336:ALA:C	1:F:338:LEU:H	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:339:GLU:O	1:D:340:GLN:C	2.56	0.44
1:A:451:VAL:HG12	1:A:451:VAL:O	2.17	0.44
1:H:438:ASN:ND2	1:H:483:SER:CB	2.80	0.44
1:B:361:PHE:O	1:B:365:ARG:HB2	2.16	0.44
1:G:354:PHE:CE2	1:G:356:TRP:HB2	2.52	0.44
1:F:355:ILE:HB	1:H:386:TYR:CE2	2.52	0.44
1:C:388:TYR:CD2	1:C:422:LEU:HD23	2.53	0.44
1:H:339:GLU:O	1:H:342:VAL:N	2.51	0.44
1:C:412:VAL:HG22	1:C:466:ALA:HB2	2.00	0.44
1:D:448:ARG:NH2	2:P:251:VAL:CG2	2.80	0.44
1:C:382:TYR:CD1	1:C:382:TYR:N	2.86	0.44
1:H:350:TYR:CD2	1:H:385:ARG:HA	2.53	0.44
1:H:414:MET:HG2	1:H:463:MET:HG2	1.99	0.43
1:F:481:LYS:O	1:F:482:ASN:HB2	2.18	0.43
1:D:363:ARG:NH1	1:D:363:ARG:HG2	2.28	0.43
1:C:476:SER:O	1:C:477:LYS:C	2.57	0.43
1:F:477:LYS:C	1:F:478:MET:O	2.55	0.43
1:C:479:GLU:O	1:C:480:ALA:O	2.36	0.43
1:A:447:PHE:CG	2:I:250:PRO:HG3	2.51	0.43
1:H:334:ALA:C	1:H:336:ALA:N	2.69	0.43
1:B:406:HIS:CD2	1:B:471:LEU:HD22	2.54	0.43
1:H:406:HIS:CE1	1:H:474:PRO:HG3	2.53	0.43
1:B:438:ASN:ND2	1:B:483:SER:CB	2.82	0.43
1:E:476:SER:O	1:E:477:LYS:O	2.36	0.43
1:E:451:VAL:CG1	1:E:451:VAL:O	2.66	0.43
1:B:478:MET:HB2	1:B:484:TYR:HB2	2.01	0.43
1:D:338:LEU:HA	1:D:338:LEU:HD12	1.82	0.43
1:D:354:PHE:CE2	1:D:356:TRP:HB2	2.54	0.43
1:C:486:ARG:HG3	1:C:486:ARG:HH11	1.84	0.43
1:H:425:PRO:HB2	3:H:1032:HOH:O	2.19	0.43
1:B:389:LYS:HG2	1:B:414:MET:CE	2.46	0.43
1:B:341:LYS:O	1:B:345:MET:HG3	2.19	0.43
1:A:476:SER:O	1:A:477:LYS:O	2.36	0.43
1:F:473:CYS:HA	1:F:474:PRO:HD3	1.87	0.43
1:D:394:ILE:CD1	1:D:407:LEU:HD21	2.49	0.43
1:E:436:ASP:OD1	1:E:483:SER:OG	2.22	0.42
1:A:469:CYS:HA	1:A:470:PRO:HD2	1.95	0.42
1:E:486:ARG:NH1	1:E:486:ARG:HG3	2.34	0.42
1:F:433:MET:HE2	1:F:444:ILE:HD12	2.00	0.42
1:B:365:ARG:NH2	1:B:397:ASN:OD1	2.52	0.42
1:G:414:MET:HG2	1:G:463:MET:HG2	2.00	0.42
1:C:425:PRO:CG	1:C:451:VAL:HG13	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:486:ARG:HG3	1:A:486:ARG:NH1	2.32	0.42
1:F:361:PHE:O	1:F:365:ARG:HB2	2.20	0.42
1:F:491:PHE:CB	3:F:1052:HOH:O	2.64	0.42
1:G:407:LEU:C	1:G:407:LEU:HD23	2.40	0.42
1:G:412:VAL:HG22	1:G:466:ALA:CB	2.50	0.42
1:D:478:MET:O	1:D:479:GLU:CB	2.68	0.42
1:E:434:LEU:HD21	1:E:478:MET:HG2	2.00	0.42
1:H:339:GLU:C	1:H:343:LEU:HD13	2.40	0.42
1:G:339:GLU:O	1:G:342:VAL:N	2.53	0.42
1:A:390:MET:HB2	1:A:390:MET:HE3	1.94	0.42
1:A:361:PHE:O	1:A:365:ARG:HB2	2.20	0.41
1:A:412:VAL:HG22	1:A:466:ALA:HB2	2.03	0.41
1:E:480:ALA:O	1:E:481:LYS:O	2.37	0.41
1:D:440:ARG:HA	1:H:441:GLU:HA	2.02	0.41
1:F:425:PRO:HG3	1:F:451:VAL:CG1	2.46	0.41
1:B:354:PHE:HE2	1:B:356:TRP:HB2	1.84	0.41
1:E:361:PHE:O	1:E:365:ARG:HB2	2.20	0.41
1:C:389:LYS:HE2	1:C:414:MET:HE3	2.02	0.41
1:F:469:CYS:HA	1:F:470:PRO:HD2	1.96	0.41
1:D:363:ARG:O	1:D:367:GLU:HG3	2.21	0.41
1:D:339:GLU:O	1:D:343:LEU:HD12	2.21	0.41
1:C:467:SER:OG	2:K:250:PRO:HB2	2.21	0.41
1:A:399:ASP:OD1	2:I:254:THR:HB	2.21	0.41
1:E:459:PRO:HG3	1:E:464:ASN:HD21	1.86	0.41
1:D:451:VAL:HA	3:D:1021:HOH:O	2.21	0.41
1:B:434:LEU:HD21	1:B:478:MET:HG2	2.02	0.41
1:G:394:ILE:CD1	1:G:407:LEU:HD21	2.48	0.40
1:E:399:ASP:OD1	2:M:254:THR:HB	2.21	0.40
1:H:486:ARG:HG3	1:H:486:ARG:NH1	2.33	0.40
1:B:473:CYS:HA	1:B:474:PRO:HD3	1.91	0.40
1:H:448:ARG:HA	1:H:449:PRO:HD3	1.91	0.40
1:G:377:PHE:CE2	1:G:463:MET:SD	3.14	0.40
1:C:467:SER:HA	2:K:252:GLN:HA	2.03	0.40
1:G:447:PHE:CG	2:O:250:PRO:HG3	2.57	0.40
1:B:418:ASN:O	1:B:422:LEU:HD13	2.22	0.40
1:F:485:VAL:HG22	1:F:490:ILE:CG2	2.51	0.40
1:F:340:GLN:HA	1:F:343:LEU:HD22	2.02	0.40
1:B:394:ILE:CD1	1:B:407:LEU:HD21	2.49	0.40
1:D:341:LYS:O	1:D:345:MET:HG3	2.22	0.40
1:B:458:ARG:HA	1:B:459:PRO:HD3	1.97	0.40
1:G:421:LEU:HD11	1:H:491:PHE:CD2	2.56	0.40
1:G:437:GLN:NE2	1:G:486:ARG:HB3	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	9	3
1	B	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	9	3
1	C	166/168 (99%)	154 (93%)	7 (4%)	5 (3%)	7	2
1	D	166/168 (99%)	156 (94%)	7 (4%)	3 (2%)	13	5
1	E	166/168 (99%)	155 (93%)	5 (3%)	6 (4%)	5	1
1	F	166/168 (99%)	158 (95%)	5 (3%)	3 (2%)	13	5
1	G	166/168 (99%)	155 (93%)	9 (5%)	2 (1%)	19	9
1	H	166/168 (99%)	152 (92%)	8 (5%)	6 (4%)	5	1
2	I	5/7 (71%)	5 (100%)	0	0	100	100
2	J	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	K	5/7 (71%)	5 (100%)	0	0	100	100
2	L	5/7 (71%)	5 (100%)	0	0	100	100
2	M	5/7 (71%)	5 (100%)	0	0	100	100
2	N	5/7 (71%)	5 (100%)	0	0	100	100
2	O	5/7 (71%)	5 (100%)	0	0	100	100
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1368/1400 (98%)	1281 (94%)	54 (4%)	33 (2%)	9	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	LYS
1	A	480	ALA
1	B	477	LYS
1	B	480	ALA
1	C	477	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	480	ALA
1	C	481	LYS
1	D	481	LYS
1	E	477	LYS
1	E	478	MET
1	E	480	ALA
1	E	481	LYS
1	F	477	LYS
1	F	480	ALA
1	H	480	ALA
1	H	482	ASN
1	D	480	ALA
1	E	479	GLU
1	G	482	ASN
1	H	335	MET
1	H	477	LYS
1	A	481	LYS
1	B	478	MET
1	E	482	ASN
1	F	478	MET
1	G	477	LYS
1	H	478	MET
1	A	479	GLU
1	B	481	LYS
1	C	478	MET
1	H	479	GLU
1	D	477	LYS
1	C	337	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/144 (92%)	128 (97%)	4 (3%)	53	50
1	B	132/144 (92%)	127 (96%)	5 (4%)	44	39
1	C	132/144 (92%)	130 (98%)	2 (2%)	76	79
1	D	132/144 (92%)	129 (98%)	3 (2%)	63	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	132/144 (92%)	129 (98%)	3 (2%)	63	63
1	F	132/144 (92%)	126 (96%)	6 (4%)	38	31
1	G	132/144 (92%)	129 (98%)	3 (2%)	63	63
1	H	132/144 (92%)	130 (98%)	2 (2%)	76	79
2	I	5/5 (100%)	4 (80%)	1 (20%)	2	1
2	J	5/5 (100%)	5 (100%)	0	100	100
2	K	5/5 (100%)	5 (100%)	0	100	100
2	L	5/5 (100%)	4 (80%)	1 (20%)	2	1
2	M	5/5 (100%)	5 (100%)	0	100	100
2	N	5/5 (100%)	4 (80%)	1 (20%)	2	1
2	O	5/5 (100%)	4 (80%)	1 (20%)	2	1
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	1096/1192 (92%)	1064 (97%)	32 (3%)	55	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	366	GLN
1	A	409	LEU
1	A	422	LEU
1	B	360	ASP
1	B	365	ARG
1	B	366	GLN
1	B	409	LEU
1	B	422	LEU
1	C	365	ARG
1	C	366	GLN
1	D	365	ARG
1	D	366	GLN
1	D	451	VAL
1	E	365	ARG
1	E	409	LEU
1	E	422	LEU
1	F	360	ASP
1	F	365	ARG
1	F	366	GLN
1	F	409	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	422	LEU
1	F	428	GLN
1	G	365	ARG
1	G	366	GLN
1	G	451	VAL
1	H	365	ARG
1	H	409	LEU
2	I	254	THR
2	L	254	THR
2	N	254	THR
2	O	254	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	HIS
1	A	461	ASN
1	B	406	HIS
1	B	438	ASN
1	B	461	ASN
1	C	406	HIS
1	C	461	ASN
1	D	406	HIS
1	D	461	ASN
1	E	366	GLN
1	E	406	HIS
1	E	418	ASN
1	E	438	ASN
1	E	461	ASN
1	F	406	HIS
1	F	461	ASN
1	G	406	HIS
1	G	438	ASN
1	G	461	ASN
1	H	366	GLN
1	H	406	HIS
1	H	438	ASN
1	H	461	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.