



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:35 PM UTC

PDB ID : 1D0A / pdb_00001d0a
Title : STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 (TRAF2)
IN COMPLEX WITH A HUMAN OX40 PEPTIDE
Authors : Ye, H.; Park, Y.C.; Kreishman, M.; Kieff, E.; Wu, H.
Deposited on : 1999-09-09
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

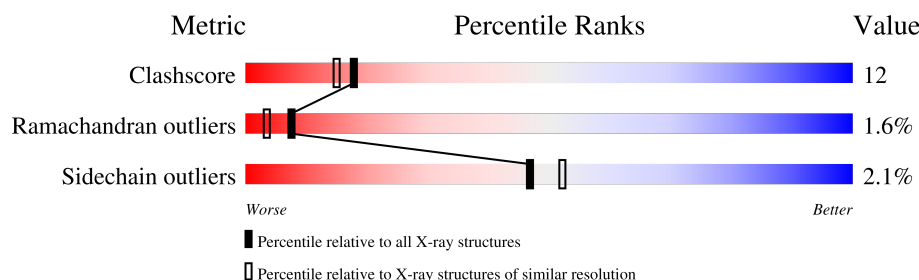
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	73% 21% 5%
1	B	168	76% 21% .
1	C	168	76% 20% .
1	D	168	66% 33% .
1	E	168	74% 24% .
1	F	168	78% 18% .
2	G	6	67% 33%
2	H	6	67% 33%

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Mol	Chain	Length	Quality of chain
2	I	6	 67% 33%
2	J	6	 67% 33%
2	K	6	 83% 17%
2	L	6	 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8683 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 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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	ARG	LEU	conflict	UNP Q12933
B	365	ARG	LEU	conflict	UNP Q12933
C	365	ARG	LEU	conflict	UNP Q12933
D	365	ARG	LEU	conflict	UNP Q12933
E	365	ARG	LEU	conflict	UNP Q12933
F	365	ARG	LEU	conflict	UNP Q12933

- Molecule 2 is a protein called OX40L RECEPTOR PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			46	28	6	12			
2	H	6	Total	C	N	O	0	0	0
			46	28	6	12			
2	I	6	Total	C	N	O	0	0	0
			46	28	6	12			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	6	Total	C	N	O	0	0	0
			46	28	6	12			
2	K	6	Total	C	N	O	0	0	0
			46	28	6	12			
2	L	6	Total	C	N	O	0	0	0
			46	28	6	12			

- Molecule 3 is water.

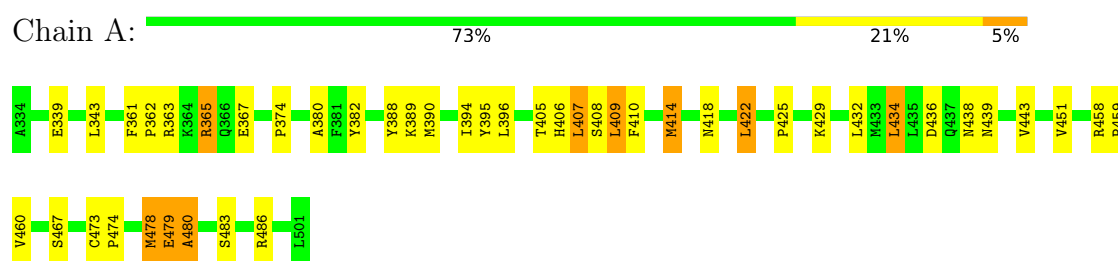
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	123	Total	O	0	0
			123	123		
3	C	124	Total	O	0	0
			124	124		
3	D	68	Total	O	0	0
			68	68		
3	E	116	Total	O	0	0
			116	116		
3	F	153	Total	O	0	0
			153	153		
3	G	4	Total	O	0	0
			4	4		
3	H	3	Total	O	0	0
			3	3		
3	I	7	Total	O	0	0
			7	7		
3	K	4	Total	O	0	0
			4	4		
3	L	4	Total	O	0	0
			4	4		

3 Residue-property plots

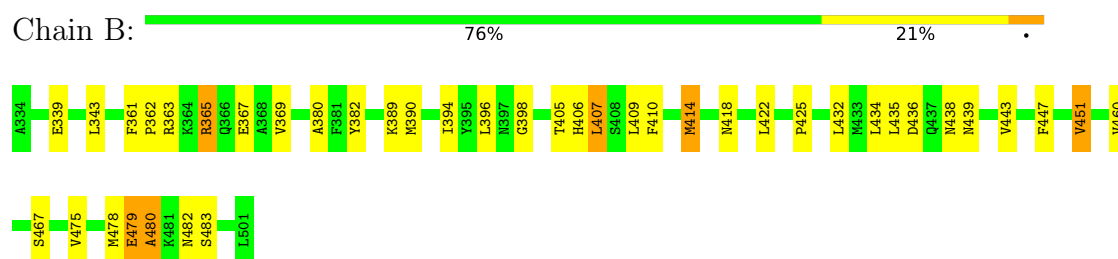
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

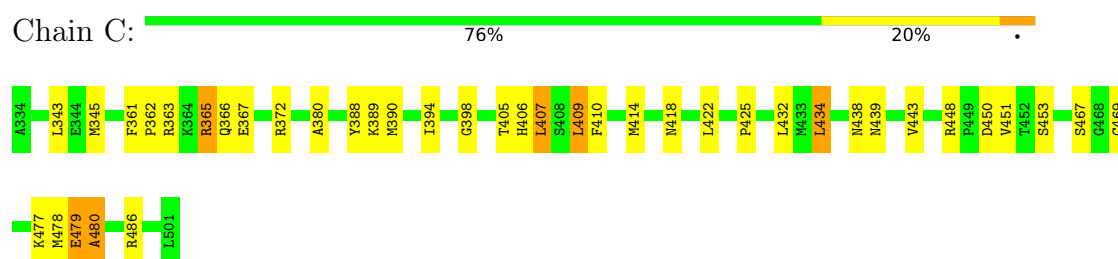
• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2



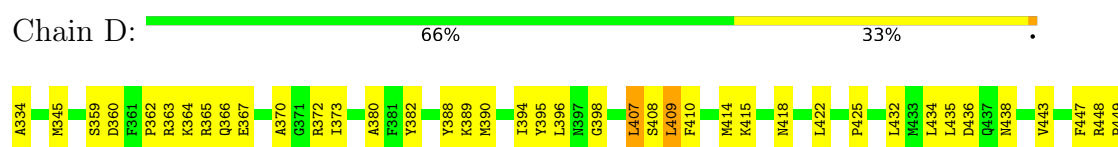
• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2



• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2



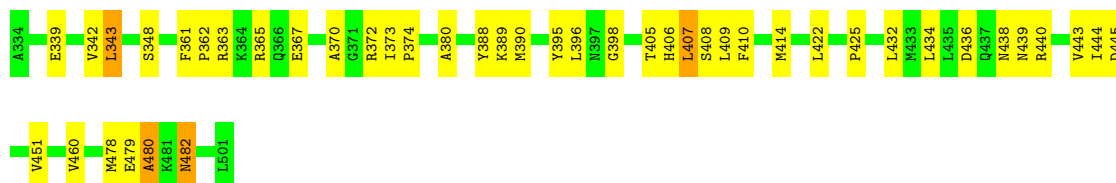
• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2





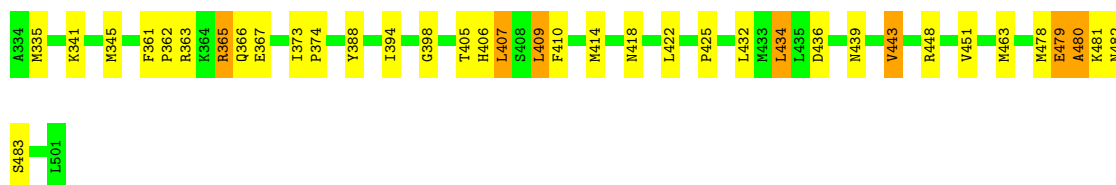
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain E: 74% 24%



- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain F: 78% 18%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain G: 67% 33%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain H: 67% 33%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain I: 67% 33%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain J: 67% 33%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain K: 83% 17%



- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain L: 83% 17%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.40Å 85.60Å 125.40Å 90.00° 118.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8683	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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

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	0.42	1/1312 (0.1%)	0.98	4/1781 (0.2%)
1	B	0.44	1/1312 (0.1%)	1.00	6/1781 (0.3%)
1	C	0.43	0/1312	1.00	5/1781 (0.3%)
1	D	0.38	0/1312	0.99	8/1781 (0.4%)
1	E	0.43	0/1312	1.00	5/1781 (0.3%)
1	F	0.43	0/1312	1.01	8/1781 (0.4%)
2	G	1.40	1/44 (2.3%)	0.85	0/58
2	H	1.39	1/44 (2.3%)	0.84	0/58
2	I	1.42	1/44 (2.3%)	0.83	0/58
2	J	1.36	1/44 (2.3%)	0.91	0/58
2	K	1.42	1/44 (2.3%)	0.86	0/58
2	L	1.38	1/44 (2.3%)	0.86	0/58
All	All	0.48	8/8136 (0.1%)	0.99	36/11034 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	261	ACE	C-N	-9.20	1.34	1.43
2	K	261	ACE	C-N	-9.14	1.34	1.43
2	G	261	ACE	C-N	-9.04	1.34	1.43
2	L	261	ACE	C-N	-8.89	1.34	1.43
2	H	261	ACE	C-N	-8.85	1.34	1.43
2	J	261	ACE	C-N	-8.80	1.34	1.43
1	A	414	MET	SD-CE	-5.08	1.66	1.79
1	B	414	MET	SD-CE	-5.05	1.67	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	GLY	N-CA-C	8.56	123.78	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	460	VAL	N-CA-C	-8.48	104.52	111.81
1	B	398	GLY	N-CA-C	8.36	122.60	112.48
1	B	460	VAL	N-CA-C	-8.11	104.85	112.96
1	F	398	GLY	N-CA-C	7.80	122.51	112.68
1	A	460	VAL	N-CA-C	-7.60	105.27	111.81
1	E	460	VAL	N-CA-C	-7.33	105.51	111.81
1	D	398	GLY	N-CA-C	7.09	121.06	112.48
1	F	407	LEU	N-CA-C	-6.97	97.89	109.46
1	E	398	GLY	N-CA-C	6.83	121.28	112.68
1	E	407	LEU	N-CA-C	-6.82	98.12	108.96
1	B	407	LEU	N-CA-C	-6.61	98.46	108.96
1	C	362	PRO	N-CA-CB	6.48	110.17	103.23
1	B	362	PRO	N-CA-CB	6.45	110.18	103.15
1	D	407	LEU	N-CA-C	-6.38	98.88	109.46
1	A	407	LEU	N-CA-C	-6.36	98.84	108.96
1	F	362	PRO	N-CA-CB	6.32	110.04	103.15
1	E	362	PRO	N-CA-CB	6.19	109.90	103.15
1	F	434	LEU	N-CA-C	-6.16	98.49	108.52
1	D	362	PRO	N-CA-CB	6.12	109.82	103.15
1	A	362	PRO	N-CA-CB	6.11	109.81	103.15
1	C	407	LEU	N-CA-C	-5.85	99.65	108.96
1	C	434	LEU	N-CA-C	-5.82	99.04	108.52
1	D	448	ARG	N-CA-C	-5.67	102.48	110.31
1	B	435	LEU	N-CA-C	5.54	118.57	109.76
1	F	373	ILE	CA-C-N	5.47	125.12	119.05
1	F	373	ILE	C-N-CA	5.47	125.12	119.05
1	F	443	VAL	N-CA-C	-5.26	101.01	108.58
1	D	435	LEU	N-CA-C	5.24	117.82	109.96
1	B	438	ASN	N-CA-C	-5.11	105.12	113.19
1	D	373	ILE	CA-C-N	5.10	124.71	119.05
1	D	373	ILE	C-N-CA	5.10	124.71	119.05
1	F	448	ARG	N-CA-C	-5.10	102.62	110.32
1	E	348	SER	N-CA-C	5.05	117.56	110.23
1	C	448	ARG	N-CA-C	-5.02	103.38	110.31
1	A	434	LEU	N-CA-C	-5.00	99.13	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1282	0	1238	36	0
1	B	1282	0	1238	31	0
1	C	1282	0	1238	29	0
1	D	1282	0	1238	38	0
1	E	1282	0	1238	34	0
1	F	1282	0	1238	26	0
2	G	46	0	41	1	0
2	H	46	0	41	1	0
2	I	46	0	41	1	0
2	J	46	0	41	1	0
2	K	46	0	41	0	0
2	L	46	0	41	0	0
3	A	109	0	0	3	0
3	B	123	0	0	1	0
3	C	124	0	0	2	0
3	D	68	0	0	1	0
3	E	116	0	0	4	0
3	F	153	0	0	5	0
3	G	4	0	0	0	0
3	H	3	0	0	0	0
3	I	7	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
All	All	8683	0	7674	193	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 12.

All (193) 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:E:389:LYS:HG2	1:E:414:MET:HE3	1.34	1.06
1:C:389:LYS:HG2	1:C:414:MET:HE3	1.35	1.05
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.39	1.04
1:B:389:LYS:HG2	1:B:414:MET:HE3	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:HG2	1:A:414:MET:HE3	1.39	1.01
1:E:425:PRO:HG3	1:E:451:VAL:HG13	1.46	0.94
1:A:425:PRO:HG3	1:A:451:VAL:HG13	1.50	0.93
1:F:425:PRO:HG3	1:F:451:VAL:HG13	1.50	0.92
1:D:436:ASP:OD1	1:D:483:SER:HB2	1.75	0.86
1:A:380:ALA:CB	1:A:414:MET:HE1	2.06	0.84
1:C:380:ALA:CB	1:C:414:MET:HE1	2.07	0.84
1:D:380:ALA:CB	1:D:414:MET:HE1	2.07	0.84
1:D:425:PRO:HG3	1:D:451:VAL:HG13	1.58	0.84
1:B:409:LEU:HD22	1:B:432:LEU:HD13	1.60	0.83
1:B:380:ALA:CB	1:B:414:MET:HE1	2.08	0.83
1:C:425:PRO:HG3	1:C:451:VAL:HG13	1.60	0.83
1:D:409:LEU:HD22	1:D:432:LEU:HD13	1.59	0.82
1:E:380:ALA:CB	1:E:414:MET:HE1	2.09	0.82
1:D:359:SER:O	1:D:364:LYS:HE2	1.79	0.82
1:B:436:ASP:OD1	1:B:483:SER:HB2	1.79	0.82
1:A:389:LYS:HG2	1:A:414:MET:CE	2.10	0.81
1:C:389:LYS:HG2	1:C:414:MET:CE	2.13	0.77
1:A:380:ALA:HB2	1:A:414:MET:HE1	1.67	0.76
1:B:380:ALA:HB2	1:B:414:MET:HE1	1.66	0.76
1:B:389:LYS:HG2	1:B:414:MET:CE	2.16	0.76
1:D:380:ALA:HB2	1:D:414:MET:HE1	1.67	0.75
1:A:436:ASP:OD1	1:A:483:SER:HB2	1.88	0.73
1:C:380:ALA:HB1	1:C:414:MET:HE1	1.71	0.71
1:E:380:ALA:HB2	1:E:414:MET:HE1	1.72	0.71
1:E:389:LYS:HG2	1:E:414:MET:CE	2.19	0.71
1:C:380:ALA:HB2	1:C:414:MET:HE1	1.74	0.69
1:A:380:ALA:HB1	1:A:414:MET:HE1	1.73	0.69
1:C:409:LEU:HD22	1:C:432:LEU:HD13	1.75	0.68
1:D:390:MET:C	1:D:414:MET:HE2	2.18	0.67
1:D:467:SER:OG	2:J:262:PRO:HB2	1.94	0.67
1:A:394:ILE:HD11	1:A:407:LEU:HD11	1.76	0.67
1:C:390:MET:C	1:C:414:MET:HE2	2.21	0.66
1:E:367:GLU:HB3	1:E:373:ILE:HD13	1.78	0.66
1:D:380:ALA:HB1	1:D:414:MET:HE1	1.77	0.65
1:E:380:ALA:HB1	1:E:414:MET:HE1	1.80	0.64
1:F:361:PHE:CZ	1:F:478:MET:HE1	2.33	0.64
1:E:390:MET:C	1:E:414:MET:HE2	2.23	0.64
1:B:425:PRO:CG	1:B:451:VAL:HG12	2.28	0.63
1:F:341:LYS:O	1:F:345:MET:HG3	1.98	0.63
1:A:425:PRO:CG	1:A:451:VAL:HG13	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:MET:HG3	1:A:479:GLU:N	2.15	0.61
1:B:380:ALA:HB1	1:B:414:MET:HE1	1.81	0.60
1:D:438:ASN:OD1	1:D:483:SER:HB3	2.01	0.60
1:E:434:LEU:HB3	1:E:443:VAL:HB	1.83	0.60
1:D:334:ALA:HB3	3:D:6478:HOH:O	2.02	0.59
1:A:438:ASN:OD1	1:A:483:SER:HB3	2.03	0.59
1:D:345:MET:SD	1:E:342:VAL:HG13	2.43	0.59
1:A:434:LEU:HB3	1:A:443:VAL:HB	1.85	0.58
1:B:407:LEU:HD22	1:B:478:MET:SD	2.44	0.58
1:C:405:THR:OG1	1:C:406:HIS:HD2	1.87	0.57
1:F:451:VAL:HG12	3:F:6508:HOH:O	2.04	0.57
1:D:363:ARG:O	1:D:367:GLU:HG3	2.03	0.57
1:B:479:GLU:O	1:B:480:ALA:C	2.48	0.57
1:B:425:PRO:HG3	1:B:451:VAL:HG12	1.87	0.56
1:E:409:LEU:HD22	1:E:432:LEU:HD13	1.86	0.56
1:F:405:THR:OG1	1:F:406:HIS:HD2	1.88	0.56
1:E:361:PHE:CZ	1:E:478:MET:HE1	2.41	0.56
1:F:481:LYS:HA	3:F:6085:HOH:O	2.04	0.56
1:B:405:THR:OG1	1:B:406:HIS:HD2	1.89	0.56
1:A:405:THR:OG1	1:A:406:HIS:HD2	1.89	0.55
1:A:361:PHE:CZ	1:A:478:MET:HE2	2.42	0.55
1:F:361:PHE:O	1:F:365:ARG:HB2	2.06	0.55
1:E:425:PRO:CG	1:E:451:VAL:HG13	2.30	0.54
1:E:482:ASN:HB3	3:E:6333:HOH:O	2.06	0.54
1:E:374:PRO:HG2	3:E:6312:HOH:O	2.07	0.54
1:C:467:SER:OG	2:I:262:PRO:HB2	2.06	0.54
1:B:478:MET:HG3	1:B:479:GLU:N	2.21	0.54
1:F:478:MET:SD	1:F:479:GLU:N	2.81	0.54
1:B:361:PHE:CZ	1:B:478:MET:HE2	2.42	0.54
1:E:339:GLU:O	1:E:343:LEU:HD22	2.07	0.54
1:B:418:ASN:O	1:B:422:LEU:HD13	2.08	0.53
1:E:396:LEU:HA	1:E:407:LEU:HD12	1.89	0.53
1:C:409:LEU:HD23	1:C:410:PHE:N	2.24	0.53
1:F:366:GLN:NE2	3:F:6264:HOH:O	2.39	0.53
1:D:396:LEU:HA	1:D:407:LEU:HD12	1.91	0.53
1:A:361:PHE:O	1:A:365:ARG:HB2	2.09	0.53
1:B:390:MET:C	1:B:414:MET:HE2	2.33	0.53
1:B:425:PRO:HG2	1:B:451:VAL:HG12	1.91	0.52
1:C:389:LYS:CG	1:C:414:MET:HE3	2.25	0.52
1:E:409:LEU:HD23	1:E:410:PHE:N	2.25	0.52
1:F:425:PRO:CG	1:F:451:VAL:HG13	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:TYR:CD2	1:D:422:LEU:HD23	2.45	0.51
1:C:479:GLU:O	1:C:480:ALA:C	2.53	0.51
1:E:372:ARG:HB3	3:E:6208:HOH:O	2.11	0.51
1:A:479:GLU:O	1:A:480:ALA:C	2.54	0.50
1:C:425:PRO:CG	1:C:451:VAL:HG13	2.37	0.50
1:D:478:MET:O	1:D:480:ALA:N	2.44	0.50
1:D:414:MET:HG2	1:D:463:MET:HG2	1.92	0.50
1:B:389:LYS:CG	1:B:414:MET:HE3	2.27	0.50
1:C:394:ILE:HD11	1:C:407:LEU:HD21	1.94	0.50
1:D:389:LYS:HG2	1:D:414:MET:CE	2.26	0.50
1:D:415:LYS:HE3	1:D:461:ASN:O	2.12	0.49
1:A:390:MET:C	1:A:414:MET:HE2	2.36	0.49
1:F:479:GLU:O	1:F:480:ALA:C	2.55	0.49
1:A:396:LEU:HA	1:A:407:LEU:HD12	1.94	0.49
1:A:418:ASN:O	1:A:422:LEU:HD13	2.12	0.49
1:C:361:PHE:O	1:C:365:ARG:HB2	2.12	0.49
1:D:366:GLN:NE2	1:D:366:GLN:HA	2.28	0.49
1:F:394:ILE:HD11	1:F:407:LEU:HD21	1.94	0.49
1:B:467:SER:OG	2:H:262:PRO:HB2	2.13	0.48
1:A:409:LEU:HD23	1:A:410:PHE:N	2.28	0.48
1:B:409:LEU:HD23	1:B:410:PHE:N	2.28	0.48
1:D:382:TYR:N	1:D:382:TYR:CD1	2.82	0.48
1:A:389:LYS:CG	1:A:414:MET:HE3	2.27	0.48
1:C:366:GLN:HE21	1:C:366:GLN:HA	1.79	0.48
1:D:395:TYR:HB2	1:D:408:SER:HB2	1.96	0.48
1:E:363:ARG:O	1:E:367:GLU:HG3	2.14	0.48
1:F:409:LEU:HD23	1:F:410:PHE:N	2.29	0.48
1:D:434:LEU:HB3	1:D:443:VAL:HB	1.96	0.47
1:F:363:ARG:O	1:F:367:GLU:HG3	2.14	0.47
1:C:366:GLN:HA	1:C:366:GLN:NE2	2.30	0.47
1:F:361:PHE:CE1	1:F:478:MET:HE1	2.49	0.47
1:F:388:TYR:CD2	1:F:422:LEU:HD23	2.50	0.47
1:D:425:PRO:CG	1:D:451:VAL:HG13	2.39	0.47
1:E:451:VAL:HG11	3:E:6712:HOH:O	2.15	0.47
1:C:372:ARG:HD2	3:C:6503:HOH:O	2.15	0.46
1:E:370:ALA:HB3	1:E:372:ARG:HD3	1.97	0.46
1:F:409:LEU:HD22	1:F:432:LEU:HD13	1.97	0.46
1:A:396:LEU:HD23	1:A:407:LEU:HD11	1.96	0.46
1:B:396:LEU:HA	1:B:407:LEU:HD12	1.97	0.46
1:C:388:TYR:CD2	1:C:422:LEU:HD23	2.51	0.46
1:E:479:GLU:O	1:E:480:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:LEU:HB3	1:C:443:VAL:HB	1.98	0.46
1:D:418:ASN:O	1:D:422:LEU:HD13	2.16	0.46
1:A:363:ARG:O	1:A:367:GLU:HG3	2.16	0.46
1:F:414:MET:HE3	1:F:463:MET:HE2	1.98	0.45
1:F:434:LEU:HB3	1:F:443:VAL:HB	1.98	0.45
1:A:467:SER:OG	2:G:262:PRO:HB2	2.16	0.45
1:C:438:ASN:OD1	1:C:486:ARG:NH2	2.50	0.45
1:D:394:ILE:HD11	1:D:407:LEU:HD11	1.97	0.45
1:A:339:GLU:O	1:A:343:LEU:HD13	2.16	0.45
1:A:382:TYR:N	1:A:382:TYR:CD1	2.84	0.45
1:C:363:ARG:O	1:C:367:GLU:HG3	2.16	0.45
1:B:434:LEU:HB3	1:B:443:VAL:HB	1.99	0.45
1:D:479:GLU:O	1:D:480:ALA:C	2.60	0.45
1:F:366:GLN:HA	1:F:366:GLN:HE21	1.81	0.45
1:E:405:THR:OG1	1:E:406:HIS:HD2	2.00	0.45
1:E:478:MET:SD	1:E:479:GLU:N	2.90	0.45
1:F:366:GLN:NE2	1:F:366:GLN:HA	2.32	0.44
1:E:388:TYR:CD2	1:E:422:LEU:HD23	2.52	0.44
3:A:6241:HOH:O	1:C:345:MET:HG3	2.17	0.44
1:A:429:LYS:HD2	3:A:6514:HOH:O	2.16	0.44
1:B:363:ARG:O	1:B:367:GLU:HG3	2.18	0.44
1:A:374:PRO:HG2	3:A:6403:HOH:O	2.18	0.43
1:E:436:ASP:C	1:E:438:ASN:H	2.26	0.43
1:D:458:ARG:HA	1:D:459:PRO:HD3	1.87	0.43
1:E:436:ASP:OD2	1:E:440:ARG:N	2.41	0.43
1:C:450:ASP:OD2	1:C:453:SER:HB2	2.18	0.43
1:B:409:LEU:HD23	1:B:409:LEU:C	2.44	0.43
1:C:418:ASN:O	1:C:422:LEU:HD13	2.19	0.43
1:A:473:CYS:HA	1:A:474:PRO:HD3	1.90	0.42
1:D:409:LEU:HD23	1:D:410:PHE:N	2.34	0.42
1:E:390:MET:O	1:E:414:MET:HE2	2.19	0.42
1:C:469:CYS:HB3	3:C:6364:HOH:O	2.19	0.42
1:E:438:ASN:HD22	1:E:438:ASN:HA	1.63	0.42
1:A:438:ASN:OD1	1:A:486:ARG:NH2	2.48	0.42
1:C:478:MET:O	1:C:480:ALA:N	2.53	0.42
1:B:365:ARG:O	1:B:369:VAL:HG23	2.20	0.42
1:F:418:ASN:O	1:F:422:LEU:HD13	2.20	0.42
1:B:394:ILE:HD11	1:B:407:LEU:HD11	2.01	0.42
1:F:374:PRO:HD2	3:F:6493:HOH:O	2.20	0.42
1:A:436:ASP:C	1:A:438:ASN:H	2.28	0.42
1:D:449:PRO:HB3	1:D:456:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:MET:HE2	1:F:478:MET:HB2	1.91	0.42
1:D:370:ALA:HB3	1:D:372:ARG:HD3	2.02	0.42
1:F:335:MET:HA	3:F:6107:HOH:O	2.19	0.42
1:D:360:ASP:HA	1:D:488:ASP:OD2	2.21	0.41
1:A:395:TYR:HB2	1:A:408:SER:HB2	2.02	0.41
1:E:444:ILE:HG12	1:E:445:ASP:N	2.35	0.41
1:F:436:ASP:OD1	1:F:483:SER:OG	2.38	0.41
1:A:458:ARG:HA	1:A:459:PRO:HD3	1.88	0.41
1:B:451:VAL:HG22	3:B:6407:HOH:O	2.20	0.41
1:E:395:TYR:HB2	1:E:408:SER:HB2	2.03	0.41
1:E:451:VAL:O	1:E:451:VAL:HG12	2.21	0.41
1:A:409:LEU:HD22	1:A:432:LEU:HD13	2.03	0.41
1:B:405:THR:O	1:B:475:VAL:HG23	2.21	0.41
1:B:447:PHE:CD1	1:B:447:PHE:C	2.99	0.41
1:B:382:TYR:CD1	1:B:382:TYR:N	2.89	0.41
1:D:474:PRO:HG2	1:D:477:LYS:HB2	2.03	0.41
1:B:339:GLU:O	1:B:343:LEU:HD13	2.21	0.40
1:D:438:ASN:OD1	1:D:486:ARG:NH2	2.49	0.40
1:A:422:LEU:CD1	1:A:422:LEU:N	2.84	0.40
1:D:365:ARG:NH2	1:D:475:VAL:CG1	2.84	0.40
1:E:367:GLU:HB3	1:E:373:ILE:CD1	2.49	0.40
1:D:390:MET:O	1:D:414:MET:HE2	2.21	0.40
1:A:388:TYR:CD2	1:A:422:LEU:HD23	2.57	0.40
1:C:361:PHE:CZ	1:C:478:MET:HE1	2.57	0.40
1:D:447:PHE:CD1	1:D:447:PHE:C	2.99	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%)	154 (93%)	8 (5%)	4 (2%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	6	3
1	C	166/168 (99%)	156 (94%)	8 (5%)	2 (1%)	10	6
1	D	126/168 (75%)	120 (95%)	6 (5%)	0	100	100
1	E	117/168 (70%)	106 (91%)	8 (7%)	3 (3%)	4	1
1	F	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	6	3
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
2	I	4/6 (67%)	4 (100%)	0	0	100	100
2	J	4/6 (67%)	4 (100%)	0	0	100	100
2	K	4/6 (67%)	4 (100%)	0	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
All	All	931/1044 (89%)	870 (93%)	46 (5%)	15 (2%)	7	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	B	480	ALA
1	C	480	ALA
1	E	480	ALA
1	F	480	ALA
1	A	439	ASN
1	A	479	GLU
1	E	439	ASN
1	C	479	GLU
1	A	478	MET
1	B	479	GLU
1	E	482	ASN
1	F	479	GLU
1	F	482	ASN
1	B	482	ASN

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	132/145 (91%)	129 (98%)	3 (2%)	44	49
1	B	132/145 (91%)	129 (98%)	3 (2%)	44	49
1	C	132/145 (91%)	127 (96%)	5 (4%)	29	29
1	D	132/145 (91%)	131 (99%)	1 (1%)	73	80
1	E	132/145 (91%)	130 (98%)	2 (2%)	57	64
1	F	132/145 (91%)	129 (98%)	3 (2%)	44	49
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	5/5 (100%)	5 (100%)	0	100	100
2	I	5/5 (100%)	5 (100%)	0	100	100
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%)	5 (100%)	0	100	100
All	All	822/900 (91%)	805 (98%)	17 (2%)	47	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	409	LEU
1	A	422	LEU
1	B	365	ARG
1	B	439	ASN
1	B	451	VAL
1	C	343	LEU
1	C	365	ARG
1	C	409	LEU
1	C	439	ASN
1	C	477	LYS
1	D	409	LEU
1	E	343	LEU
1	E	365	ARG
1	F	365	ARG
1	F	409	LEU
1	F	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	HIS
1	A	461	ASN
1	B	406	HIS
1	B	461	ASN
1	C	366	GLN
1	C	406	HIS
1	C	461	ASN
1	D	366	GLN
1	D	406	HIS
1	D	439	ASN
1	D	461	ASN
1	E	406	HIS
1	E	418	ASN
1	E	437	GLN
1	E	439	ASN
1	E	461	ASN
1	F	366	GLN
1	F	406	HIS
1	F	438	ASN
1	F	439	ASN

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 oligosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.