Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:20 PM EDT

PDB ID	:	1D0A
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 (i) 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 (i)) were used in the production of this report:

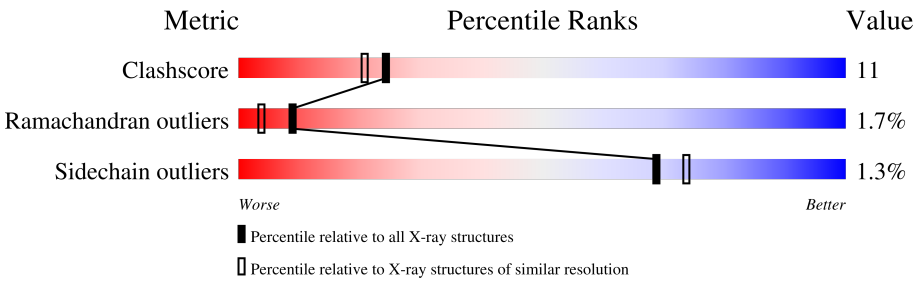
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	74% 23% •
1	B	168	80% 18% •
1	C	168	80% 18% •
1	D	168	69% 29% •
1	E	168	77% 22% •
1	F	168	82% 16% •
2	G	6	83% 17%
2	H	6	83% 17%

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Mol	Chain	Length	Quality of chain
2	I	6	83% 17%
2	J	6	83% 17%
2	K	6	100%
2	L	6	100%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	168	1282	825	217	231	9	0	0	0
1	B	168	1282	825	217	231	9	0	0	0
1	C	168	1282	825	217	231	9	0	0	0
1	D	168	1282	825	217	231	9	0	0	0
1	E	168	1282	825	217	231	9	0	0	0
1	F	168	1282	825	217	231	9	0	0	0

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
			Total	C	N	O			
2	G	6	46	28	6	12	0	0	0
2	H	6	46	28	6	12	0	0	0
2	I	6	46	28	6	12	0	0	0

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

- Molecule 3 is water.

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

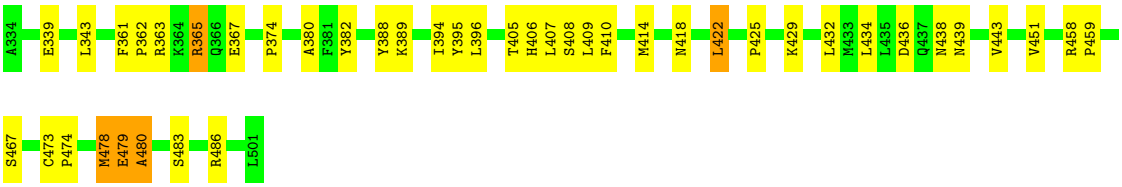
3 Residue-property plots (i)

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. 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.

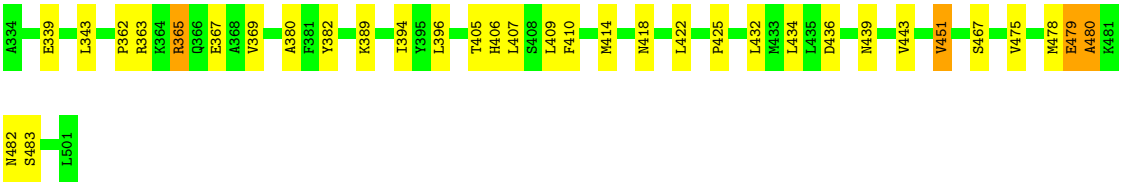
• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain A:



• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain B:

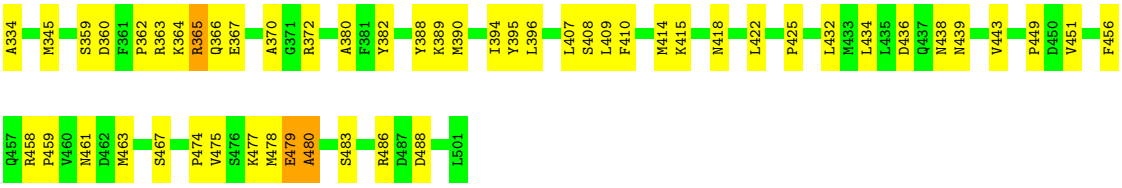


• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain C:

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain D:



• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain E: 77% 22%

A334 E339 V342 L343 P362 R363 K364 R365 Q366 E367 A370 G371 R372 I373 P374 Y388 K389 M390 Y395 L396 T405 H406 L407 S408 L409 F410 M414 L422 P425 L432 M433 L434 L435 D436 Q437 N438 N439 R440 V443 I444 D445 V451 M478 E479 A480 K481 N482 L501

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain F: 82% 16%

A334 M335 K341 M345 F361 P362 R363 K364 R365 Q366 E367 P374 Y388 I394 T405 H406 L407 S408 L409 F410 N418 L422 P425 L432 M433 L434 N439 V443 V451 M478 E479 A480 K481 N482 L501

• Molecule 2: OX40L RECEPTOR PEPTIDE

Chain G: 83% 17%

ACE261 P262 E266

• Molecule 2: OX40L RECEPTOR PEPTIDE

Chain H: 83% 17%

ACE261 P262 E266

• Molecule 2: OX40L RECEPTOR PEPTIDE

Chain I: 83% 17%

ACE261 P262 E266

• Molecule 2: OX40L RECEPTOR PEPTIDE

Chain J: 83% 17%

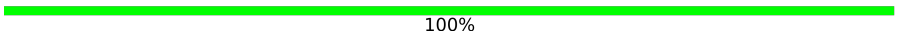
ACE261 P262 E266

• Molecule 2: OX40L RECEPTOR PEPTIDE

Chain K: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: OX40L RECEPTOR PEPTIDE

Chain L: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.35	0/1312	0.68	1/1781 (0.1%)
1	B	0.37	0/1312	0.69	1/1781 (0.1%)
1	C	0.37	0/1312	0.68	1/1781 (0.1%)
1	D	0.35	0/1312	0.67	1/1781 (0.1%)
1	E	0.36	0/1312	0.69	1/1781 (0.1%)
1	F	0.37	0/1312	0.69	1/1781 (0.1%)
2	G	0.36	0/44	0.68	0/58
2	H	0.36	0/44	0.66	0/58
2	I	0.34	0/44	0.66	0/58
2	J	0.32	0/44	0.70	0/58
2	K	0.34	0/44	0.72	0/58
2	L	0.35	0/44	0.68	0/58
All	All	0.36	0/8136	0.68	6/11034 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	362	PRO	N-CA-CB	5.74	110.18	103.30
1	C	362	PRO	N-CA-CB	5.72	110.17	103.30
1	F	362	PRO	N-CA-CB	5.62	110.04	103.30
1	E	362	PRO	N-CA-CB	5.50	109.90	103.30
1	D	362	PRO	N-CA-CB	5.43	109.82	103.30
1	A	362	PRO	N-CA-CB	5.43	109.81	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1282	0	1238	34	0
1	B	1282	0	1238	27	0
1	C	1282	0	1238	26	0
1	D	1282	0	1238	35	0
1	E	1282	0	1238	30	0
1	F	1282	0	1238	21	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	172	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 11.

All (172) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:389:LYS:HG2	1:A:414:MET:HE3	1.60	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:HE3	1.63	0.81
1:C:389:LYS:HG2	1:C:414:MET:CE	2.13	0.77
1:B:389:LYS:HG2	1:B:414:MET:HE3	1.66	0.77
1:B:389:LYS:HG2	1:B:414:MET:CE	2.16	0.76
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.66	0.75
1:E:389:LYS:HG2	1:E:414:MET:HE3	1.67	0.75
1:B:389:LYS:HE2	1:B:414:MET:HE3	1.68	0.74
1:A:436:ASP:OD1	1:A:483:SER:HB2	1.88	0.73
1:E:389:LYS:HG2	1:E:414:MET:CE	2.19	0.71
1:A:389:LYS:HE2	1:A:414:MET:HE3	1.73	0.69
1:C:409:LEU:HD22	1:C:432:LEU:HD13	1.75	0.68
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:E:367:GLU:HB3	1:E:373:ILE:HD13	1.78	0.66
1:D:389:LYS:HG2	1:D:414:MET:CE	2.26	0.65
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
1:C:389:LYS:HE2	1:C:414:MET:HE3	1.82	0.62
1:A:478:MET:HG3	1:A:479:GLU:N	2.15	0.61
1:E:389:LYS:HE2	1:E:414:MET:HE3	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:THR:OG1	1:F:406:HIS:HD2	1.88	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: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:B:478:MET:HG3	1:B:479:GLU:N	2.21	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:D:389:LYS:HE2	1:D:414:MET:HE3	1.88	0.54
1:F:478:MET:SD	1:F:479:GLU:N	2.81	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:A:380:ALA:CB	1:A:414:MET:HE1	2.39	0.53
1:B:425:PRO:HG2	1:B:451:VAL:HG12	1.91	0.52
1:C:389:LYS:HG2	1:C:414:MET:HE2	1.92	0.52
1:E:409:LEU:HD23	1:E:410:PHE:N	2.25	0.52
1:B:479:GLU:O	1:B:480:ALA:C	2.48	0.52
1:F:425:PRO:CG	1:F:451:VAL:HG13	2.31	0.52
1:D:388:TYR:CD2	1:D:422:LEU:HD23	2.45	0.51
1:E:372:ARG:HB3	3:E:6208:HOH:O	2.11	0.51
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:C:394:ILE:HD11	1:C:407:LEU:HD21	1.94	0.50
1:D:415:LYS:HE3	1:D:461:ASN:O	2.12	0.49
1:B:380:ALA:CB	1:B:414:MET:HE1	2.42	0.49
1:C:390:MET:O	1:C:414:MET:HE1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:388:TYR:CD2	1:F:422:LEU:HD23	2.50	0.47
1:C:479:GLU:O	1:C:480:ALA:C	2.53	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: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:B:389:LYS:HG2	1:B:414:MET:HE2	1.95	0.46
1:A:479:GLU:O	1:A:480:ALA:C	2.54	0.46
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:F:366:GLN:HA	1:F:366:GLN:HE21	1.81	0.45
1:E:390:MET:O	1:E:414:MET:HE1	2.17	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:F:479:GLU:O	1:F:480:ALA:C	2.55	0.44
1:E:388:TYR:CD2	1:E:422:LEU:HD23	2.52	0.44
1:E:389:LYS:HG2	1:E:414:MET:HE2	1.97	0.44
3:A:6241:HOH:O	1:C:345:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:458:ARG:HA	1:D:459:PRO:HD3	1.87	0.43
1:A:389:LYS:CG	1:A:414:MET:HE3	2.40	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:C:418:ASN:O	1:C:422:LEU:HD13	2.19	0.43
1:A:389:LYS:HG2	1:A:414:MET:HE2	1.93	0.42
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:B:389:LYS:CE	1:B:414:MET:HE3	2.45	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:D:449:PRO:HB3	1:D:456:PHE:CD2	2.55	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:A:380:ALA:HB1	1:A:414:MET:HE1	2.02	0.41
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:E:479:GLU:O	1:E:480:ALA:C	2.58	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:D:390:MET:O	1:D:414:MET:HE1	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:GLU:O	1:D:480:ALA:C	2.60	0.40
1:E:367:GLU:HB3	1:E:373:ILE:CD1	2.49	0.40
1:D:380:ALA:CB	1:D:414:MET:HE1	2.51	0.40
1:A:388:TYR:CD2	1:A:422:LEU:HD23	2.57	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	166/168 (99%)	154 (93%)	8 (5%)	4 (2%)	6	2
1	B	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	3
1	C	166/168 (99%)	156 (94%)	8 (5%)	2 (1%)	13	7
1	D	166/168 (99%)	153 (92%)	11 (7%)	2 (1%)	13	7
1	E	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	3
1	F	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	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	1020/1044 (98%)	952 (93%)	51 (5%)	17 (2%)	9	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	B	480	ALA
1	C	480	ALA
1	D	480	ALA
1	E	480	ALA
1	F	480	ALA
1	A	439	ASN
1	A	479	GLU
1	D	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 (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	132/145 (91%)	130 (98%)	2 (2%)	65	69
1	B	132/145 (91%)	129 (98%)	3 (2%)	50	53
1	C	132/145 (91%)	131 (99%)	1 (1%)	81	86
1	D	132/145 (91%)	130 (98%)	2 (2%)	65	69
1	E	132/145 (91%)	131 (99%)	1 (1%)	81	86
1	F	132/145 (91%)	130 (98%)	2 (2%)	65	69
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	5/5 (100%)	5 (100%)	0	100	100
All	All	822/900 (91%)	811 (99%)	11 (1%)	69	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	422	LEU
1	B	365	ARG
1	B	439	ASN
1	B	451	VAL
1	C	365	ARG
1	D	365	ARG
1	D	439	ASN
1	E	365	ARG
1	F	365	ARG
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	438	ASN
1	E	461	ASN
1	F	366	GLN
1	F	406	HIS
1	F	438	ASN
1	F	439	ASN
1	F	461	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.