



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:16 PM UTC

PDB ID : 1RF3 / pdb_00001rf3
Title : Structurally Distinct Recognition Motifs in Lymphotoxin-B Receptor and CD40 for TRAF-mediated Signaling
Authors : Li, C.; Norris, P.S.; Ni, C.Z.; Havert, M.L.; Chiong, E.M.; Tran, B.R.; Cabezas, E.; Cheng, G.; Reed, J.C.; Satterthwait, A.C.; Ware, C.F.; Ely, K.R.
Deposited on : 2003-11-07
Resolution : 3.50 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) : **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

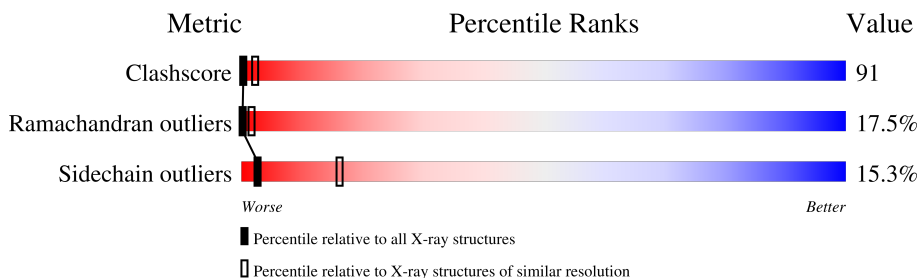
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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	200	15% 54% 26% • •
2	B	24	12% 42% 42% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1709 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 TNF receptor associated factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1531	979	259	282	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	LEU	-	expression tag	UNP Q13114
A	506	GLU	-	expression tag	UNP Q13114
A	507	HIS	-	expression tag	UNP Q13114
A	508	HIS	-	expression tag	UNP Q13114
A	509	HIS	-	expression tag	UNP Q13114
A	510	HIS	-	expression tag	UNP Q13114
A	511	HIS	-	expression tag	UNP Q13114
A	512	HIS	-	expression tag	UNP Q13114

- Molecule 2 is a protein called 24-residue peptide from Lymphotoxin-B Receptor.

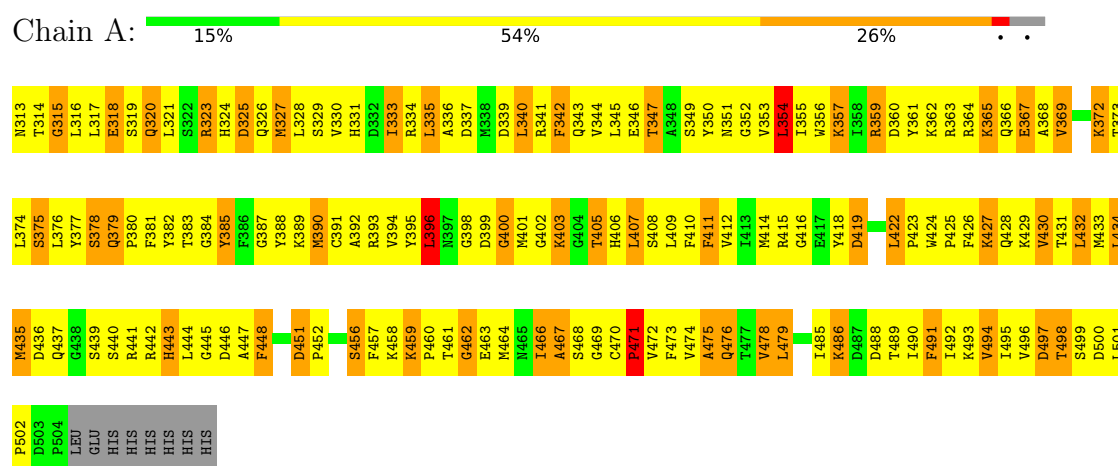
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	0	0	0
			178	111	28	39			

3 Residue-property plots

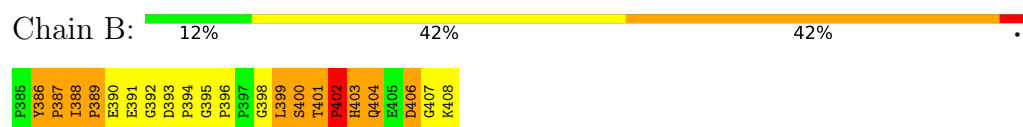
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: TNF receptor associated factor 3



- Molecule 2: 24-residue peptide from Lymphotoxin-B Receptor



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.70Å 83.70Å 79.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.50	Depositor
% Data completeness (in resolution range)	83.0 (8.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.266 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1709	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/1566	1.08	13/2113 (0.6%)
2	B	0.63	0/186	1.41	5/254 (2.0%)
All	All	0.55	0/1752	1.12	18/2367 (0.8%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	LYS	CA-C-N	8.81	128.89	119.90
1	A	459	LYS	C-N-CA	8.81	128.89	119.90
1	A	333	ILE	N-CA-C	-7.38	104.54	111.48
1	A	443	HIS	N-CA-C	7.20	119.52	109.15
2	B	395	GLY	CA-C-N	6.34	126.91	120.38
2	B	395	GLY	C-N-CA	6.34	126.91	120.38
2	B	396	PRO	CA-C-N	6.16	126.96	120.12
2	B	396	PRO	C-N-CA	6.16	126.96	120.12
1	A	327	MET	N-CA-C	-6.14	103.89	111.75
1	A	347	THR	N-CA-C	-6.09	105.16	112.59
2	B	388	ILE	N-CA-C	5.61	121.01	108.88
1	A	340	LEU	N-CA-C	-5.51	105.27	111.28
1	A	418	TYR	N-CA-C	-5.35	106.80	113.38
1	A	411	PHE	N-CA-C	-5.34	102.10	110.17
1	A	378	SER	N-CA-C	5.32	116.37	108.60
1	A	325	ASP	N-CA-C	5.18	117.01	111.36
1	A	475	ALA	N-CA-C	5.13	117.10	109.25
1	A	318	GLU	N-CA-C	-5.02	106.32	112.90

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	1531	0	1526	283	0
2	B	178	0	158	40	0
All	All	1709	0	1684	309	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 91.

All (309) 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:A:406:HIS:HA	1:A:476:GLN:HG2	1.32	1.11
1:A:323:ARG:HH11	1:A:323:ARG:HB3	1.21	1.02
1:A:399:ASP:HA	1:A:403:LYS:HD2	1.39	1.01
1:A:409:LEU:HD12	1:A:410:PHE:H	1.30	0.97
1:A:432:LEU:HA	1:A:494:VAL:HA	1.47	0.96
1:A:390:MET:HE3	1:A:496:VAL:HG21	1.50	0.94
1:A:398:GLY:O	1:A:403:LYS:HA	1.70	0.89
2:B:390:GLU:OE1	2:B:391:GLU:N	2.06	0.89
1:A:467:ALA:HB3	2:B:391:GLU:OE2	1.73	0.88
1:A:323:ARG:HB3	1:A:323:ARG:NH1	1.89	0.88
1:A:406:HIS:HB2	1:A:475:ALA:HA	1.53	0.87
1:A:409:LEU:HD12	1:A:410:PHE:N	1.89	0.86
1:A:430:VAL:HA	1:A:495:ILE:O	1.77	0.85
1:A:486:LYS:NZ	1:A:486:LYS:HB3	1.92	0.84
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.43	0.83
1:A:498:THR:O	1:A:501:LEU:HB3	1.78	0.82
1:A:324:HIS:O	1:A:328:LEU:HB2	1.80	0.81
1:A:475:ALA:O	1:A:478:VAL:HG22	1.80	0.81
1:A:474:VAL:CG1	1:A:479:LEU:HB2	2.11	0.80
1:A:419:ASP:HA	1:A:422:LEU:HD22	1.62	0.80
1:A:434:LEU:HG	1:A:474:VAL:HG21	1.62	0.79
1:A:408:SER:HG	1:A:410:PHE:HE1	1.27	0.79
1:A:429:LYS:O	1:A:496:VAL:HA	1.83	0.78
2:B:403:HIS:CG	2:B:404:GLN:H	2.01	0.78
1:A:406:HIS:CA	1:A:476:GLN:HG2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:HD3	1:A:459:LYS:C	2.10	0.77
1:A:391:CYS:O	1:A:412:VAL:HG12	1.84	0.77
1:A:389:LYS:HE2	1:A:414:MET:SD	2.25	0.77
1:A:357:LYS:HE3	1:A:489:THR:CG2	2.16	0.76
1:A:315:GLY:HA2	1:A:318:GLU:OE2	1.86	0.75
2:B:387:PRO:O	2:B:388:ILE:HG22	1.86	0.75
1:A:463:GLU:O	1:A:464:MET:HG2	1.86	0.75
1:A:399:ASP:OD1	2:B:392:GLY:HA3	1.88	0.74
1:A:342:PHE:O	1:A:346:GLU:HB2	1.88	0.73
1:A:393:ARG:HG2	1:A:395:TYR:HE1	1.54	0.72
1:A:368:ALA:HA	1:A:373:THR:O	1.89	0.72
1:A:320:GLN:HA	1:A:320:GLN:HE21	1.55	0.71
1:A:406:HIS:HA	1:A:476:GLN:CG	2.18	0.71
1:A:432:LEU:HB3	1:A:494:VAL:HG12	1.73	0.71
2:B:386:TYR:HD2	2:B:387:PRO:HD2	1.56	0.71
1:A:359:ARG:HG3	1:A:359:ARG:NH1	2.01	0.70
1:A:344:VAL:HG23	1:A:345:LEU:H	1.55	0.70
1:A:434:LEU:O	1:A:443:HIS:HB2	1.91	0.70
1:A:354:LEU:HD22	1:A:355:ILE:N	2.07	0.70
1:A:407:LEU:C	1:A:407:LEU:HD23	2.17	0.69
1:A:366:GLN:HA	1:A:369:VAL:HG13	1.74	0.69
1:A:367:GLU:HG2	1:A:372:LYS:HD2	1.75	0.69
1:A:320:GLN:HE21	1:A:320:GLN:CA	2.07	0.68
1:A:407:LEU:HD23	1:A:408:SER:N	2.08	0.68
1:A:474:VAL:HG12	1:A:479:LEU:HB2	1.76	0.68
1:A:353:VAL:HG22	1:A:354:LEU:H	1.58	0.67
1:A:362:LYS:O	1:A:365:LYS:HB3	1.94	0.67
2:B:398:GLY:HA3	2:B:402:PRO:HG2	1.76	0.67
1:A:490:ILE:O	1:A:490:ILE:HD12	1.94	0.67
1:A:399:ASP:OD1	1:A:400:GLY:N	2.28	0.67
1:A:406:HIS:HE1	1:A:472:VAL:HG22	1.60	0.67
2:B:389:PRO:O	2:B:390:GLU:HB2	1.95	0.66
1:A:356:TRP:CZ2	1:A:377:TYR:O	2.49	0.66
1:A:391:CYS:CB	1:A:414:MET:HE3	2.26	0.65
1:A:469:GLY:O	1:A:471:PRO:HD3	1.96	0.65
1:A:356:TRP:CH2	1:A:394:VAL:HG12	2.31	0.65
1:A:396:LEU:CD2	1:A:396:LEU:H	2.09	0.65
1:A:407:LEU:HB3	1:A:474:VAL:O	1.97	0.65
1:A:406:HIS:CB	1:A:475:ALA:HA	2.24	0.65
1:A:415:ARG:HD3	1:A:462:GLY:O	1.96	0.65
1:A:382:TYR:CE2	1:A:389:LYS:HG3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASP:HA	1:A:403:LYS:CD	2.23	0.64
1:A:356:TRP:CD2	1:A:378:SER:HB3	2.33	0.64
1:A:354:LEU:HD22	1:A:355:ILE:H	1.62	0.64
1:A:437:GLN:HG3	1:A:486:LYS:HG3	1.80	0.63
1:A:497:ASP:O	1:A:498:THR:HB	1.98	0.63
1:A:471:PRO:CD	2:B:389:PRO:HB2	2.29	0.62
2:B:390:GLU:CD	2:B:391:GLU:H	2.06	0.62
1:A:428:GLN:HE21	1:A:497:ASP:HB3	1.64	0.62
1:A:360:ASP:O	1:A:364:ARG:HD3	1.99	0.62
2:B:403:HIS:CG	2:B:404:GLN:N	2.66	0.61
1:A:444:LEU:HD23	1:A:445:GLY:N	2.14	0.61
1:A:432:LEU:HD23	1:A:446:ASP:O	2.00	0.61
2:B:388:ILE:HG23	2:B:388:ILE:O	2.01	0.61
1:A:372:LYS:HG3	1:A:373:THR:N	2.16	0.61
1:A:345:LEU:O	1:A:345:LEU:HD23	2.00	0.61
1:A:471:PRO:HD2	2:B:389:PRO:HG2	1.82	0.61
1:A:398:GLY:C	1:A:403:LYS:HA	2.26	0.60
1:A:359:ARG:HH11	1:A:359:ARG:CG	2.13	0.60
1:A:426:PHE:HB3	1:A:457:PHE:HB3	1.82	0.60
1:A:425:PRO:HB3	1:A:458:LYS:HA	1.82	0.60
1:A:387:GLY:C	1:A:422:LEU:HD21	2.27	0.59
1:A:415:ARG:NE	1:A:463:GLU:OE2	2.35	0.59
1:A:432:LEU:CB	1:A:494:VAL:HG12	2.33	0.59
1:A:363:ARG:HD2	1:A:367:GLU:OE2	2.02	0.59
1:A:382:TYR:HE2	1:A:389:LYS:HG3	1.68	0.59
1:A:388:TYR:CE2	1:A:422:LEU:HG	2.38	0.59
1:A:409:LEU:C	1:A:410:PHE:CD1	2.81	0.59
1:A:405:THR:OG1	1:A:406:HIS:N	2.36	0.58
1:A:470:CYS:HA	2:B:389:PRO:HD2	1.83	0.58
1:A:486:LYS:HB3	1:A:486:LYS:HZ2	1.66	0.58
2:B:388:ILE:N	2:B:389:PRO:HD3	2.18	0.58
1:A:431:THR:HA	1:A:447:ALA:HB2	1.85	0.58
1:A:434:LEU:CG	1:A:474:VAL:HG21	2.33	0.58
1:A:372:LYS:HG3	1:A:373:THR:H	1.67	0.58
1:A:499:SER:C	1:A:501:LEU:H	2.11	0.58
1:A:313:ASN:C	1:A:315:GLY:H	2.12	0.57
1:A:314:THR:O	1:A:316:LEU:N	2.37	0.57
1:A:471:PRO:HD2	2:B:389:PRO:CG	2.34	0.57
1:A:333:ILE:O	1:A:336:ALA:HB3	2.05	0.57
1:A:365:LYS:HG3	1:A:366:GLN:N	2.19	0.57
1:A:396:LEU:H	1:A:396:LEU:HD23	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:HIS:CB	1:A:476:GLN:H	2.16	0.57
1:A:463:GLU:C	1:A:464:MET:HG2	2.30	0.57
1:A:416:GLY:CA	1:A:419:ASP:HB2	2.34	0.57
1:A:486:LYS:HB3	1:A:486:LYS:HZ3	1.68	0.57
1:A:435:MET:C	1:A:443:HIS:HB3	2.30	0.57
1:A:356:TRP:HH2	1:A:394:VAL:H	1.53	0.56
2:B:386:TYR:CD2	2:B:387:PRO:HD2	2.39	0.56
1:A:410:PHE:HA	1:A:469:GLY:HA3	1.87	0.56
1:A:344:VAL:HG23	1:A:345:LEU:N	2.21	0.56
1:A:366:GLN:O	1:A:368:ALA:N	2.38	0.56
1:A:426:PHE:CB	1:A:457:PHE:HB3	2.35	0.56
1:A:315:GLY:HA2	1:A:318:GLU:CD	2.30	0.56
1:A:391:CYS:C	1:A:412:VAL:HG12	2.31	0.56
2:B:406:ASP:CG	2:B:407:GLY:H	2.13	0.56
1:A:430:VAL:CA	1:A:495:ILE:O	2.52	0.56
1:A:430:VAL:HG23	1:A:430:VAL:O	2.06	0.56
1:A:320:GLN:HA	1:A:320:GLN:NE2	2.20	0.56
1:A:474:VAL:HG11	1:A:479:LEU:HB2	1.87	0.55
1:A:497:ASP:O	1:A:498:THR:CB	2.54	0.55
1:A:402:GLY:O	1:A:403:LYS:C	2.49	0.55
2:B:401:THR:H	2:B:402:PRO:HD2	1.71	0.55
1:A:388:TYR:OH	1:A:423:PRO:HD2	2.07	0.55
1:A:391:CYS:SG	1:A:392:ALA:N	2.80	0.55
1:A:414:MET:HA	1:A:464:MET:HA	1.88	0.55
1:A:356:TRP:CE3	1:A:392:ALA:HB3	2.42	0.55
1:A:381:PHE:HD1	1:A:381:PHE:H	1.55	0.54
1:A:380:PRO:HG3	1:A:414:MET:HE1	1.90	0.54
1:A:354:LEU:O	1:A:355:ILE:HD13	2.08	0.54
1:A:451:ASP:OD2	2:B:388:ILE:HG12	2.07	0.54
1:A:340:LEU:C	1:A:342:PHE:H	2.16	0.53
1:A:327:MET:O	1:A:330:VAL:HB	2.08	0.53
1:A:472:VAL:HG11	2:B:407:GLY:N	2.24	0.53
1:A:490:ILE:HD12	1:A:490:ILE:C	2.34	0.53
1:A:336:ALA:HA	1:A:339:ASP:OD2	2.09	0.53
1:A:347:THR:HB	1:A:379:GLN:OE1	2.08	0.53
1:A:448:PHE:HB3	2:B:387:PRO:CG	2.38	0.53
1:A:491:PHE:N	1:A:491:PHE:CD1	2.77	0.52
1:A:499:SER:O	1:A:501:LEU:N	2.36	0.52
2:B:398:GLY:C	2:B:400:SER:H	2.16	0.52
1:A:330:VAL:HG12	1:A:331:HIS:HD2	1.74	0.52
1:A:395:TYR:O	1:A:396:LEU:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TYR:HB3	1:A:488:ASP:OD2	2.09	0.52
1:A:475:ALA:O	1:A:476:GLN:C	2.53	0.52
1:A:351:ASN:OD1	1:A:353:VAL:HG12	2.10	0.51
1:A:431:THR:O	1:A:495:ILE:HG12	2.10	0.51
1:A:395:TYR:O	1:A:398:GLY:N	2.43	0.51
1:A:393:ARG:HG2	1:A:395:TYR:CE1	2.39	0.51
1:A:463:GLU:C	1:A:464:MET:CG	2.84	0.51
1:A:361:TYR:O	1:A:365:LYS:N	2.34	0.50
1:A:357:LYS:HE3	1:A:489:THR:HG21	1.91	0.50
1:A:458:LYS:O	1:A:459:LYS:C	2.55	0.50
1:A:471:PRO:HD2	2:B:389:PRO:HB2	1.91	0.50
1:A:407:LEU:C	1:A:407:LEU:CD2	2.83	0.50
1:A:456:SER:OG	1:A:468:SER:HB2	2.11	0.50
1:A:357:LYS:HE3	1:A:489:THR:HG23	1.93	0.50
1:A:433:MET:HA	1:A:473:PHE:HZ	1.76	0.50
1:A:493:LYS:HG2	1:A:495:ILE:HD11	1.93	0.50
1:A:498:THR:HG23	1:A:499:SER:N	2.26	0.50
1:A:356:TRP:CZ2	1:A:394:VAL:HG12	2.46	0.50
1:A:365:LYS:O	1:A:368:ALA:HB3	2.12	0.50
1:A:351:ASN:OD1	1:A:351:ASN:C	2.54	0.50
1:A:357:LYS:HD3	1:A:491:PHE:CE2	2.47	0.50
2:B:402:PRO:O	2:B:403:HIS:HB2	2.12	0.50
1:A:376:LEU:HB2	1:A:394:VAL:HG12	1.93	0.50
1:A:416:GLY:HA3	1:A:419:ASP:HB2	1.94	0.50
1:A:356:TRP:HA	1:A:379:GLN:HE22	1.77	0.49
1:A:350:TYR:O	1:A:384:GLY:N	2.45	0.49
1:A:428:GLN:NE2	1:A:497:ASP:HB3	2.26	0.49
1:A:408:SER:OG	1:A:410:PHE:HE1	1.89	0.49
1:A:314:THR:C	1:A:316:LEU:H	2.20	0.49
1:A:376:LEU:HB2	1:A:394:VAL:CG1	2.42	0.49
1:A:343:GLN:O	1:A:344:VAL:C	2.54	0.49
1:A:364:ARG:HG3	1:A:364:ARG:HH11	1.78	0.49
1:A:360:ASP:HA	1:A:488:ASP:OD1	2.12	0.49
1:A:412:VAL:HG23	1:A:467:ALA:HA	1.94	0.49
1:A:336:ALA:O	1:A:339:ASP:HB2	2.12	0.48
1:A:499:SER:C	1:A:501:LEU:N	2.69	0.48
1:A:337:ASP:C	1:A:339:ASP:H	2.21	0.48
1:A:314:THR:C	1:A:316:LEU:N	2.71	0.48
1:A:353:VAL:O	1:A:354:LEU:CB	2.61	0.48
2:B:401:THR:HB	2:B:402:PRO:HD3	1.94	0.48
1:A:376:LEU:O	1:A:393:ARG:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:HD3	1:A:460:PRO:N	2.28	0.48
1:A:427:LYS:C	1:A:428:GLN:HG2	2.37	0.48
1:A:437:GLN:CD	1:A:486:LYS:HB2	2.38	0.48
1:A:433:MET:N	1:A:493:LYS:O	2.43	0.47
1:A:334:ARG:C	1:A:336:ALA:N	2.68	0.47
1:A:398:GLY:O	1:A:403:LYS:HD2	2.14	0.47
1:A:387:GLY:O	1:A:422:LEU:HD21	2.14	0.47
1:A:356:TRP:HE3	1:A:392:ALA:HB3	1.76	0.47
1:A:374:LEU:O	1:A:375:SER:HB2	2.15	0.47
1:A:391:CYS:N	1:A:412:VAL:O	2.48	0.47
1:A:448:PHE:C	1:A:448:PHE:CD2	2.91	0.47
1:A:366:GLN:C	1:A:368:ALA:N	2.72	0.47
1:A:448:PHE:C	1:A:448:PHE:HD2	2.22	0.47
1:A:334:ARG:O	1:A:336:ALA:N	2.47	0.47
1:A:391:CYS:HB2	1:A:414:MET:HE3	1.96	0.46
1:A:431:THR:HB	1:A:495:ILE:CG1	2.44	0.46
1:A:459:LYS:HA	1:A:460:PRO:HD3	1.79	0.46
1:A:351:ASN:OD1	1:A:352:GLY:N	2.48	0.46
1:A:353:VAL:O	1:A:354:LEU:HB2	2.15	0.46
2:B:398:GLY:HA3	2:B:402:PRO:CG	2.45	0.46
1:A:340:LEU:HA	1:A:343:GLN:OE1	2.16	0.46
1:A:349:SER:HB3	1:A:381:PHE:HB2	1.98	0.46
1:A:406:HIS:HB3	1:A:476:GLN:H	1.80	0.46
1:A:343:GLN:O	1:A:347:THR:N	2.48	0.46
1:A:366:GLN:O	1:A:369:VAL:HG13	2.16	0.46
1:A:471:PRO:HD2	2:B:389:PRO:CB	2.45	0.46
2:B:406:ASP:C	2:B:408:LYS:H	2.22	0.46
1:A:366:GLN:HA	1:A:369:VAL:CG1	2.43	0.46
1:A:366:GLN:O	1:A:367:GLU:C	2.58	0.46
2:B:398:GLY:CA	2:B:402:PRO:HG2	2.45	0.46
1:A:394:VAL:HG22	1:A:395:TYR:N	2.31	0.46
1:A:467:ALA:HB3	2:B:391:GLU:CD	2.39	0.46
2:B:406:ASP:CG	2:B:407:GLY:N	2.74	0.46
1:A:485:ILE:HA	1:A:490:ILE:CG2	2.46	0.46
1:A:424:TRP:HB3	1:A:425:PRO:HA	1.99	0.45
1:A:437:GLN:HG3	1:A:486:LYS:CG	2.45	0.45
1:A:406:HIS:HA	1:A:476:GLN:HE21	1.82	0.45
1:A:431:THR:HB	1:A:495:ILE:HB	1.97	0.45
1:A:407:LEU:HD12	1:A:479:LEU:CD2	2.47	0.45
2:B:399:LEU:O	2:B:400:SER:CB	2.65	0.45
1:A:334:ARG:O	1:A:335:LEU:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TRP:HA	1:A:379:GLN:NE2	2.31	0.45
1:A:436:ASP:HB2	1:A:443:HIS:HB3	1.98	0.45
1:A:430:VAL:HG21	1:A:448:PHE:CE2	2.52	0.45
1:A:377:TYR:OH	1:A:393:ARG:CZ	2.64	0.45
1:A:415:ARG:HG2	1:A:463:GLU:HA	1.99	0.45
1:A:444:LEU:HD23	1:A:445:GLY:H	1.79	0.45
1:A:353:VAL:HG13	1:A:354:LEU:N	2.31	0.44
1:A:496:VAL:HG12	1:A:497:ASP:N	2.32	0.44
1:A:318:GLU:HA	1:A:321:LEU:HB2	1.98	0.44
1:A:320:GLN:O	1:A:321:LEU:C	2.59	0.44
1:A:331:HIS:C	1:A:333:ILE:H	2.23	0.44
1:A:470:CYS:O	1:A:471:PRO:C	2.61	0.44
1:A:344:VAL:C	1:A:346:GLU:H	2.26	0.44
1:A:367:GLU:HB3	1:A:372:LYS:HG3	1.99	0.44
1:A:407:LEU:HD23	1:A:408:SER:O	2.17	0.44
1:A:466:ILE:O	1:A:467:ALA:C	2.61	0.44
1:A:325:ASP:O	1:A:328:LEU:HB3	2.18	0.44
1:A:337:ASP:C	1:A:339:ASP:N	2.75	0.44
1:A:377:TYR:OH	1:A:393:ARG:NH1	2.51	0.44
1:A:383:THR:HG23	1:A:390:MET:SD	2.58	0.44
1:A:433:MET:HA	1:A:473:PHE:CZ	2.53	0.44
1:A:432:LEU:CA	1:A:494:VAL:HA	2.34	0.43
1:A:409:LEU:HG	1:A:432:LEU:HD12	2.00	0.43
1:A:316:LEU:O	1:A:319:SER:N	2.51	0.43
1:A:396:LEU:CD2	1:A:396:LEU:N	2.77	0.43
1:A:353:VAL:O	1:A:381:PHE:HD2	2.01	0.43
1:A:491:PHE:N	1:A:491:PHE:HD1	2.17	0.43
1:A:367:GLU:CG	1:A:372:LYS:HD2	2.44	0.43
1:A:329:SER:O	1:A:333:ILE:HG12	2.19	0.43
1:A:399:ASP:O	1:A:400:GLY:C	2.61	0.43
1:A:408:SER:OG	1:A:471:PRO:HA	2.19	0.43
1:A:440:SER:HB3	1:A:442:ARG:HH21	1.84	0.43
1:A:473:PHE:CD2	1:A:474:VAL:HG23	2.54	0.43
2:B:403:HIS:CD2	2:B:404:GLN:H	2.35	0.43
2:B:388:ILE:O	2:B:388:ILE:HG13	2.19	0.43
2:B:392:GLY:O	2:B:393:ASP:C	2.62	0.42
1:A:315:GLY:C	1:A:318:GLU:OE1	2.62	0.42
1:A:330:VAL:O	1:A:333:ILE:HB	2.19	0.42
1:A:359:ARG:O	1:A:360:ASP:HB2	2.19	0.42
1:A:485:ILE:HA	1:A:490:ILE:HG22	2.00	0.42
1:A:356:TRP:CE3	1:A:378:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:SER:OG	1:A:410:PHE:CE1	2.70	0.42
2:B:391:GLU:OE1	2:B:391:GLU:HA	2.19	0.42
1:A:385:TYR:N	1:A:385:TYR:CD2	2.86	0.42
1:A:416:GLY:H	1:A:419:ASP:CB	2.32	0.42
1:A:466:ILE:HG22	2:B:391:GLU:HB3	2.01	0.42
1:A:354:LEU:C	1:A:354:LEU:HD13	2.45	0.42
1:A:356:TRP:CE2	1:A:377:TYR:O	2.72	0.42
1:A:402:GLY:HA2	1:A:405:THR:CG2	2.49	0.42
1:A:498:THR:CG2	1:A:499:SER:N	2.83	0.42
1:A:331:HIS:C	1:A:333:ILE:N	2.78	0.42
1:A:434:LEU:CB	1:A:474:VAL:HG21	2.49	0.42
1:A:366:GLN:O	1:A:369:VAL:N	2.53	0.41
1:A:422:LEU:HA	1:A:423:PRO:HD3	1.77	0.41
1:A:347:THR:OG1	1:A:379:GLN:HG2	2.20	0.41
1:A:459:LYS:HD3	1:A:460:PRO:O	2.20	0.41
1:A:314:THR:O	1:A:317:LEU:N	2.48	0.41
1:A:407:LEU:HD23	1:A:408:SER:C	2.45	0.41
1:A:424:TRP:CG	1:A:459:LYS:HB2	2.55	0.41
1:A:451:ASP:HA	1:A:452:PRO:HD2	1.83	0.41
2:B:399:LEU:O	2:B:400:SER:OG	2.35	0.41
1:A:345:LEU:O	1:A:345:LEU:CD2	2.67	0.41
1:A:350:TYR:CD1	1:A:350:TYR:N	2.87	0.41
1:A:355:ILE:HD11	1:A:493:LYS:HD2	2.03	0.41
1:A:374:LEU:O	1:A:375:SER:CB	2.68	0.41
1:A:384:GLY:O	1:A:385:TYR:C	2.62	0.41
1:A:459:LYS:C	1:A:459:LYS:CD	2.84	0.41
1:A:315:GLY:HA2	1:A:318:GLU:OE1	2.20	0.41
1:A:340:LEU:HA	1:A:343:GLN:NE2	2.35	0.41
1:A:326:GLN:C	1:A:328:LEU:N	2.75	0.41
1:A:410:PHE:HE2	2:B:390:GLU:C	2.28	0.41
1:A:466:ILE:O	1:A:468:SER:N	2.54	0.41
1:A:375:SER:OG	1:A:393:ARG:NH2	2.51	0.41
1:A:390:MET:HB3	1:A:411:PHE:CZ	2.56	0.41
1:A:431:THR:CA	1:A:447:ALA:HB2	2.50	0.41
1:A:361:TYR:CD1	1:A:361:TYR:C	2.99	0.40
1:A:394:VAL:HG22	1:A:396:LEU:HD22	2.02	0.40
1:A:409:LEU:C	1:A:410:PHE:HD1	2.29	0.40
1:A:411:PHE:O	1:A:412:VAL:HB	2.22	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	190/200 (95%)	125 (66%)	38 (20%)	27 (14%)	0	3
2	B	22/24 (92%)	8 (36%)	4 (18%)	10 (46%)	0	0
All	All	212/224 (95%)	133 (63%)	42 (20%)	37 (18%)	0	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	SER
1	A	385	TYR
1	A	439	SER
1	A	471	PRO
1	A	476	GLN
2	B	389	PRO
2	B	400	SER
2	B	402	PRO
1	A	315	GLY
1	A	354	LEU
1	A	367	GLU
1	A	396	LEU
1	A	427	LYS
1	A	456	SER
1	A	466	ILE
1	A	467	ALA
1	A	498	THR
2	B	387	PRO
2	B	401	THR
2	B	403	HIS
2	B	404	GLN
2	B	406	ASP
1	A	365	LYS
1	A	405	THR
1	A	435	MET

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Mol	Chain	Res	Type
1	A	497	ASP
1	A	502	PRO
2	B	399	LEU
1	A	341	ARG
1	A	400	GLY
1	A	430	VAL
1	A	335	LEU
1	A	419	ASP
1	A	500	ASP
1	A	403	LYS
1	A	462	GLY
2	B	394	PRO

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	169/177 (96%)	142 (84%)	27 (16%)	2	14
2	B	20/20 (100%)	18 (90%)	2 (10%)	7	28
All	All	189/197 (96%)	160 (85%)	29 (15%)	3	16

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	A	323	ARG
1	A	342	PHE
1	A	354	LEU
1	A	357	LYS
1	A	359	ARG
1	A	369	VAL
1	A	372	LYS
1	A	379	GLN
1	A	390	MET
1	A	396	LEU

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Mol	Chain	Res	Type
1	A	401	MET
1	A	407	LEU
1	A	422	LEU
1	A	432	LEU
1	A	434	LEU
1	A	441	ARG
1	A	448	PHE
1	A	451	ASP
1	A	461	THR
1	A	471	PRO
1	A	478	VAL
1	A	479	LEU
1	A	486	LYS
1	A	491	PHE
1	A	492	ILE
1	A	494	VAL
2	B	386	TYR
2	B	402	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	A	320	GLN
1	A	331	HIS
1	A	366	GLN
1	A	379	GLN
1	A	406	HIS
1	A	428	GLN
1	A	443	HIS
1	A	476	GLN
2	B	404	GLN

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 [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

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.