



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2026 – 03:11 PM JST

PDB ID : 44LS / pdb_000044ls
Title : Crystal structure of the fusion protein of T-lineage protein Themis and adaptor protein Grb2
Authors : Ouyang, S.; Zhao, Y.
Deposited on : 2026-08-03
Resolution : 3.06 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 Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

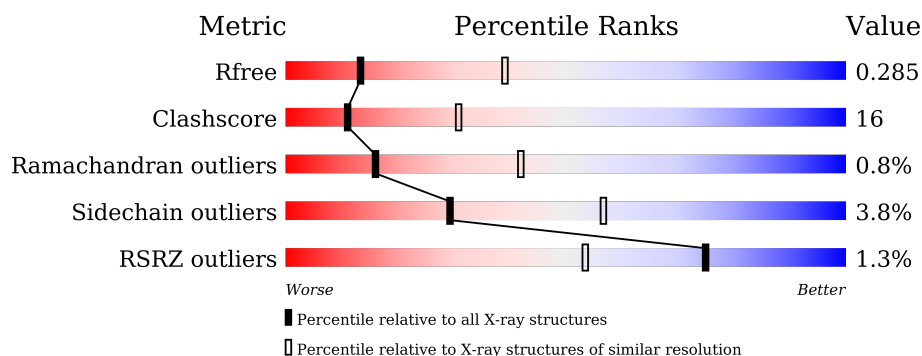
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	648	% 52% 26% • 19%
1	B	648	% 51% 27% •• 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8522 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 Protein THEMIS, Growth factor receptor-bound protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	521	Total	C	N	O	S	0	0	0
			4204	2702	706	777	19			
1	A	527	Total	C	N	O	S	0	0	0
			4276	2754	714	788	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	initiating methionine	UNP Q8N1K5
B	-22	HIS	-	expression tag	UNP Q8N1K5
B	-21	HIS	-	expression tag	UNP Q8N1K5
B	-20	HIS	-	expression tag	UNP Q8N1K5
B	-19	HIS	-	expression tag	UNP Q8N1K5
B	-18	HIS	-	expression tag	UNP Q8N1K5
B	-17	HIS	-	expression tag	UNP Q8N1K5
B	-16	SER	-	expression tag	UNP Q8N1K5
B	-15	SER	-	expression tag	UNP Q8N1K5
B	-14	GLY	-	expression tag	UNP Q8N1K5
B	-13	VAL	-	expression tag	UNP Q8N1K5
B	-12	ASP	-	expression tag	UNP Q8N1K5
B	-11	LEU	-	expression tag	UNP Q8N1K5
B	-10	GLY	-	expression tag	UNP Q8N1K5
B	-9	THR	-	expression tag	UNP Q8N1K5
B	-8	GLU	-	expression tag	UNP Q8N1K5
B	-7	ASN	-	expression tag	UNP Q8N1K5
B	-6	LEU	-	expression tag	UNP Q8N1K5
B	-5	TYR	-	expression tag	UNP Q8N1K5
B	-4	PHE	-	expression tag	UNP Q8N1K5
B	-3	GLN	-	expression tag	UNP Q8N1K5
B	-2	SER	-	expression tag	UNP Q8N1K5
B	-1	ASN	-	expression tag	UNP Q8N1K5
B	0	ALA	-	expression tag	UNP Q8N1K5
B	562	GLY	-	linker	UNP Q8N1K5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	563	GLY	-	linker	UNP Q8N1K5
B	564	SER	-	linker	UNP Q8N1K5
B	565	GLY	-	linker	UNP Q8N1K5
B	566	GLY	-	linker	UNP Q8N1K5
B	567	SER	-	linker	UNP Q8N1K5
A	-23	MET	-	initiating methionine	UNP Q8N1K5
A	-22	HIS	-	expression tag	UNP Q8N1K5
A	-21	HIS	-	expression tag	UNP Q8N1K5
A	-20	HIS	-	expression tag	UNP Q8N1K5
A	-19	HIS	-	expression tag	UNP Q8N1K5
A	-18	HIS	-	expression tag	UNP Q8N1K5
A	-17	HIS	-	expression tag	UNP Q8N1K5
A	-16	SER	-	expression tag	UNP Q8N1K5
A	-15	SER	-	expression tag	UNP Q8N1K5
A	-14	GLY	-	expression tag	UNP Q8N1K5
A	-13	VAL	-	expression tag	UNP Q8N1K5
A	-12	ASP	-	expression tag	UNP Q8N1K5
A	-11	LEU	-	expression tag	UNP Q8N1K5
A	-10	GLY	-	expression tag	UNP Q8N1K5
A	-9	THR	-	expression tag	UNP Q8N1K5
A	-8	GLU	-	expression tag	UNP Q8N1K5
A	-7	ASN	-	expression tag	UNP Q8N1K5
A	-6	LEU	-	expression tag	UNP Q8N1K5
A	-5	TYR	-	expression tag	UNP Q8N1K5
A	-4	PHE	-	expression tag	UNP Q8N1K5
A	-3	GLN	-	expression tag	UNP Q8N1K5
A	-2	SER	-	expression tag	UNP Q8N1K5
A	-1	ASN	-	expression tag	UNP Q8N1K5
A	0	ALA	-	expression tag	UNP Q8N1K5
A	562	GLY	-	linker	UNP Q8N1K5
A	563	GLY	-	linker	UNP Q8N1K5
A	564	SER	-	linker	UNP Q8N1K5
A	565	GLY	-	linker	UNP Q8N1K5
A	566	GLY	-	linker	UNP Q8N1K5
A	567	SER	-	linker	UNP Q8N1K5

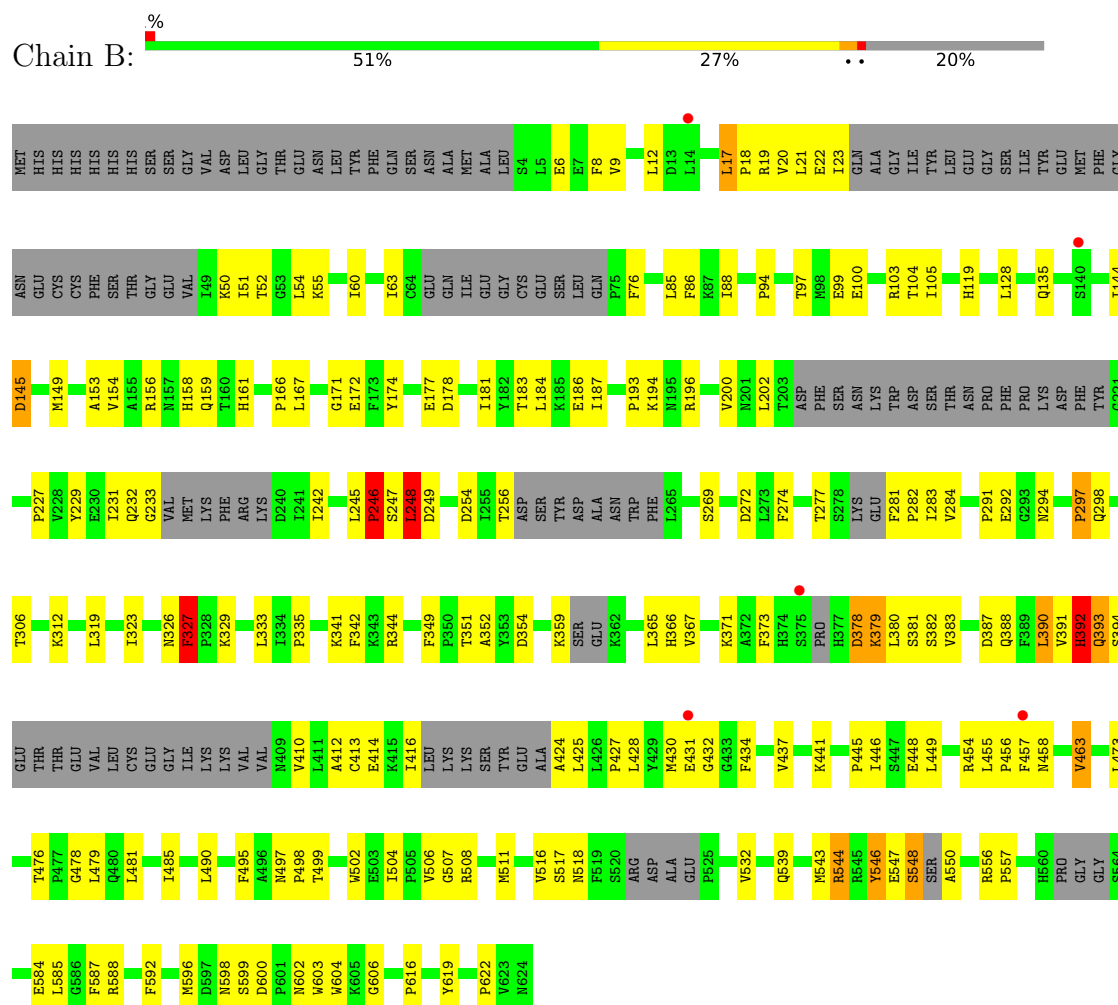
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	18	Total O 18 18	0	0
2	A	24	Total O 24 24	0	0

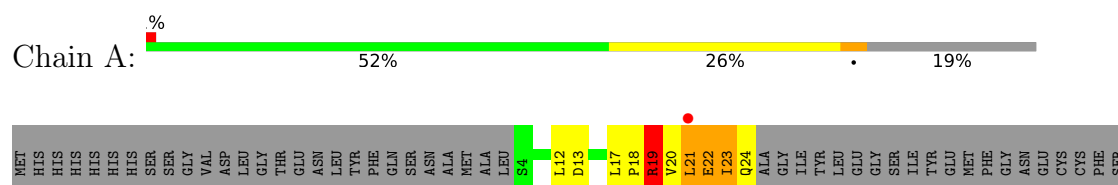
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protein THEMIS,Growth factor receptor-bound protein 2



- Molecule 1: Protein THEMIS,Growth factor receptor-bound protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.80Å 136.54Å 116.52Å 90.00° 112.61° 90.00°	Depositor
Resolution (Å)	35.94 – 3.06 35.94 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.94-3.06) 97.7 (35.94-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.06Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.260 , 0.286 0.260 , 0.285	Depositor DCC
R_{free} test set	1341 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtrriage
Anisotropy	0.635	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8522	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7472e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/4373	0.85	7/5913 (0.1%)
1	B	0.51	0/4295	0.85	7/5805 (0.1%)
All	All	0.52	0/8668	0.85	14/11718 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	499	THR	N-CA-C	-7.06	105.29	114.04
1	B	392	HIS	N-CA-C	-6.81	105.30	112.93
1	A	496	ALA	N-CA-C	6.74	125.15	110.80
1	B	498	PRO	CB-CA-C	6.67	122.56	111.56
1	B	499	THR	N-CA-C	6.42	118.85	111.02
1	A	609	HIS	CB-CA-C	-5.77	109.90	116.54
1	A	498	PRO	N-CA-CB	-5.74	97.22	103.25
1	A	170	GLU	CB-CA-C	-5.70	101.31	114.41
1	A	190	TRP	CA-C-O	-5.68	115.00	121.58
1	B	248	LEU	N-CA-C	-5.62	98.84	110.80
1	B	390	LEU	N-CA-C	-5.52	101.08	108.86
1	A	190	TRP	N-CA-C	-5.24	101.44	109.41
1	B	327	PHE	CA-C-N	-5.12	113.43	119.84
1	B	327	PHE	C-N-CA	-5.12	113.43	119.84

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Sidechain
1	A	281	PHE	Peptide
1	B	281	PHE	Peptide
1	B	327	PHE	Peptide
1	B	344	ARG	Sidechain
1	B	544	ARG	Sidechain

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	4276	0	4287	146	0
1	B	4204	0	4205	144	0
2	A	24	0	0	7	0
2	B	18	0	0	2	0
All	All	8522	0	8492	278	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 16.

All (278) 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:97:THR:HG23	1:A:100:GLU:H	1.36	0.91
1:A:235:MET:HA	2:A:705:HOH:O	1.76	0.84
1:B:394:SER:CB	1:B:412:ALA:H	1.93	0.80
1:B:341:LYS:HB2	1:B:463:VAL:HG13	1.65	0.78
1:A:23:ILE:HG23	1:A:252:VAL:HA	1.65	0.77
1:A:327:PHE:O	1:A:328:PRO:C	2.29	0.75
1:B:392:HIS:N	1:B:413:CYS:SG	2.61	0.73
1:B:274:PHE:O	1:B:312:LYS:NZ	2.22	0.73
1:B:392:HIS:H	1:B:413:CYS:HB2	1.53	0.73
1:A:12:LEU:O	1:A:194:LYS:NZ	2.22	0.72
1:A:574:LEU:HD11	1:A:621:THR:HB	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ARG:NH2	1:A:584:GLU:OE2	2.22	0.71
1:A:279:LYS:H	1:A:279:LYS:HZ2	1.38	0.71
1:B:156:ARG:HB2	1:B:161:HIS:CE1	2.27	0.70
1:B:97:THR:HG23	1:B:100:GLU:H	1.57	0.69
1:B:598:ASN:ND2	1:A:597:ASP:OD1	2.23	0.69
1:A:390:LEU:HD22	1:A:392:HIS:CE1	2.28	0.69
1:B:584:GLU:OE2	1:A:556:ARG:NH2	2.25	0.69
1:A:365:LEU:HB2	1:A:391:VAL:HB	1.73	0.69
1:B:88:ILE:HD12	1:B:178:ASP:OD2	1.94	0.68
1:A:377:HIS:HB2	2:A:719:HOH:O	1.93	0.68
1:B:149:MET:HE2	1:B:166:PRO:HB3	1.75	0.67
1:A:205:PHE:HB2	2:A:710:HOH:O	1.93	0.67
1:A:276:MET:HG3	1:A:280:GLU:HB3	1.75	0.67
1:A:86:PHE:CE1	1:A:202:LEU:HD13	2.30	0.66
1:A:508:ARG:NH2	2:A:701:HOH:O	2.25	0.65
1:B:596:MET:HE2	1:B:606:GLY:HA2	1.78	0.65
1:B:365:LEU:H	1:B:391:VAL:HG22	1.62	0.65
1:B:231:ILE:HG13	1:B:246:PRO:HD3	1.78	0.65
1:B:445:PRO:HG2	1:B:448:GLU:HG2	1.81	0.63
1:B:100:GLU:O	1:B:104:THR:HG22	2.00	0.62
1:B:119:HIS:NE2	1:B:171:GLY:HA3	2.14	0.62
1:A:500:GLU:HG3	1:A:527:LEU:HD23	1.81	0.62
1:A:125:LEU:HD23	1:A:126:GLU:H	1.64	0.61
1:A:248:LEU:HB2	2:A:720:HOH:O	1.99	0.61
1:A:345:ARG:HD2	1:A:346:PRO:HD2	1.83	0.61
1:B:193:PRO:HG2	1:B:196:ARG:HB2	1.83	0.60
1:B:366:HIS:NE2	1:B:416:ILE:HG13	2.17	0.60
1:B:388:GLN:HB2	1:B:416:ILE:HB	1.82	0.60
1:A:335:PRO:HD2	1:A:532:VAL:HG12	1.84	0.60
1:A:142:GLU:O	1:A:148:ILE:HG13	2.02	0.60
1:A:300:ILE:HG22	1:A:307:ILE:HG22	1.84	0.60
1:A:440:ASP:HB2	2:A:712:HOH:O	2.02	0.59
1:B:245:LEU:O	1:B:246:PRO:C	2.45	0.59
1:B:327:PHE:HA	1:B:329:LYS:HG3	1.83	0.59
1:A:243:ARG:HH22	1:A:289:GLU:CD	2.10	0.59
1:A:119:HIS:NE2	1:A:171:GLY:HA3	2.18	0.59
1:B:413:CYS:O	1:B:424:ALA:N	2.36	0.59
1:A:472:VAL:HG12	1:A:532:VAL:HG23	1.84	0.59
1:A:17:LEU:HG	1:A:18:PRO:HD3	1.84	0.58
1:B:507:GLY:C	1:B:508:ARG:HG2	2.27	0.58
1:B:392:HIS:O	1:B:393:GLN:C	2.46	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG22	1:A:354:ASP:OD2	2.03	0.58
1:A:116:CYS:SG	1:A:137:MET:HG2	2.44	0.58
1:B:55:LYS:HD3	1:B:232:GLN:HE22	1.68	0.57
1:A:23:ILE:HG13	1:A:24:GLN:N	2.17	0.57
1:A:366:HIS:ND1	1:A:437:VAL:HB	2.19	0.57
1:A:327:PHE:O	1:A:329:LYS:N	2.38	0.57
1:B:455:LEU:HB2	1:B:456:PRO:HD3	1.86	0.56
1:B:85:LEU:HD12	1:B:181:ILE:HG22	1.88	0.56
1:B:86:PHE:CE2	1:B:202:LEU:HD13	2.40	0.56
1:B:390:LEU:HG	1:B:416:ILE:HD11	1.88	0.56
1:A:440:ASP:CB	2:A:712:HOH:O	2.53	0.56
1:B:6:GLU:OE1	1:B:248:LEU:HB2	2.07	0.55
1:B:365:LEU:H	1:B:391:VAL:CG2	2.19	0.55
1:A:204:ASP:CG	1:A:205:PHE:H	2.15	0.55
1:A:235:MET:O	1:A:235:MET:HG2	2.06	0.55
1:B:431:GLU:HB2	1:A:601:PRO:HG3	1.87	0.55
1:A:269:SER:H	1:A:272:ASP:CG	2.15	0.55
1:B:349:PHE:HB2	1:B:434:PHE:HB2	1.89	0.54
1:B:441:LYS:CB	2:B:718:HOH:O	2.55	0.54
1:A:291:PRO:HG3	1:A:511:MET:HB3	1.90	0.54
1:A:344:ARG:HH22	1:A:347:ARG:CZ	2.21	0.54
1:B:291:PRO:HG3	1:B:511:MET:HB2	1.90	0.54
1:B:366:HIS:ND1	1:B:437:VAL:HG11	2.22	0.54
1:A:17:LEU:HG	1:A:18:PRO:CD	2.38	0.53
1:A:125:LEU:HD23	1:A:126:GLU:N	2.22	0.53
1:A:454:ARG:NE	1:A:454:ARG:HA	2.23	0.53
1:A:276:MET:CG	1:A:280:GLU:HB3	2.39	0.53
1:B:410:VAL:HG21	1:B:425:LEU:HD12	1.90	0.53
1:B:490:LEU:HG	1:B:506:VAL:HG22	1.91	0.53
1:A:597:ASP:HB3	1:A:605:LYS:HB3	1.91	0.53
1:B:50:LYS:O	1:B:233:GLY:HA3	2.08	0.53
1:B:247:SER:OG	1:B:249:ASP:HB2	2.08	0.53
1:A:17:LEU:HD23	1:A:17:LEU:H	1.74	0.53
1:B:86:PHE:CE1	1:B:184:LEU:HB2	2.44	0.52
1:B:598:ASN:OD1	1:A:597:ASP:HA	2.08	0.52
1:B:441:LYS:HB2	2:B:718:HOH:O	2.08	0.52
1:A:13:ASP:HB2	1:A:103:ARG:HD3	1.92	0.52
1:A:576:ASP:HB3	1:A:588:ARG:HH21	1.75	0.52
1:B:367:VAL:HG11	1:B:434:PHE:HB3	1.92	0.52
1:A:576:ASP:HB3	1:A:588:ARG:NH2	2.24	0.52
1:A:596:MET:HE2	1:A:606:GLY:HA2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:PHE:O	1:B:588:ARG:NH1	2.43	0.51
1:A:488:SER:O	1:A:506:VAL:HG22	2.10	0.51
1:A:539:GLN:O	1:A:543:MET:HG2	2.09	0.51
1:B:153:ALA:HA	1:B:161:HIS:O	2.11	0.51
1:B:378:ASP:C	1:B:380:LEU:N	2.69	0.51
1:A:241:ILE:HG22	1:A:243:ARG:HG3	1.91	0.51
1:A:473:LEU:HD11	1:A:479:LEU:HD11	1.93	0.50
1:B:94:PRO:HB3	1:B:174:TYR:CE2	2.46	0.50
1:A:112:LEU:HD13	1:A:545:ARG:NH1	2.26	0.50
1:B:454:ARG:O	1:B:457:PHE:HD1	1.95	0.50
1:B:456:PRO:HA	1:B:481:LEU:O	2.11	0.50
1:A:430:MET:HG3	1:A:430:MET:O	2.11	0.50
1:B:158:HIS:O	1:B:159:GLN:NE2	2.42	0.50
1:A:21:LEU:HD11	1:A:51:ILE:HD11	1.94	0.50
1:B:392:HIS:H	1:B:413:CYS:CB	2.23	0.50
1:A:119:HIS:HE2	1:A:171:GLY:HA3	1.77	0.49
1:A:149:MET:HG2	1:A:166:PRO:HA	1.94	0.49
1:A:269:SER:O	1:A:270:THR:C	2.55	0.49
1:B:602:ASN:OD1	1:A:351:THR:HG21	2.12	0.49
1:B:622:PRO:HB2	1:A:327:PHE:HZ	1.76	0.49
1:B:105:ILE:CD1	1:B:193:PRO:HB3	2.42	0.49
1:B:297:PRO:HD2	1:B:504:ILE:HD11	1.94	0.49
1:A:119:HIS:CD2	1:A:123:ILE:HD11	2.48	0.49
1:B:387:ASP:OD1	1:B:388:GLN:N	2.45	0.49
1:B:60:ILE:HG23	1:B:76:PHE:O	2.13	0.49
1:A:459:VAL:HG22	1:A:481:LEU:HD13	1.94	0.49
1:A:119:HIS:HD2	1:A:173:PHE:CE1	2.31	0.49
1:A:511:MET:HE2	1:A:513:VAL:CG1	2.42	0.48
1:B:392:HIS:HB2	1:B:413:CYS:SG	2.53	0.48
1:A:611:GLN:HG2	1:A:612:THR:H	1.79	0.48
1:B:449:LEU:HB3	1:B:457:PHE:CZ	2.47	0.48
1:B:616:PRO:HB2	1:B:619:TYR:CD1	2.49	0.48
1:A:273:LEU:O	1:A:276:MET:HB3	2.13	0.48
1:A:611:GLN:HG2	1:A:612:THR:N	2.28	0.48
1:B:319:LEU:HG	1:B:485:ILE:HD13	1.95	0.48
1:A:21:LEU:HA	1:A:253:LYS:O	2.14	0.48
1:A:349:PHE:HB2	1:A:434:PHE:HB2	1.96	0.48
1:B:135:GLN:O	1:B:154:VAL:HG12	2.14	0.48
1:B:247:SER:O	1:B:249:ASP:N	2.45	0.48
1:B:449:LEU:HB3	1:B:457:PHE:CE2	2.49	0.48
1:A:271:GLU:O	1:A:272:ASP:C	2.54	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PRO:HG2	1:A:509:LEU:HD23	1.96	0.48
1:B:54:LEU:HD21	1:B:229:TYR:HB3	1.96	0.47
1:B:413:CYS:SG	1:B:414:GLU:N	2.87	0.47
1:A:23:ILE:HG12	1:A:251:GLU:O	2.13	0.47
1:A:343:LYS:NZ	1:A:441:LYS:NZ	2.63	0.47
1:B:231:ILE:HD11	1:B:246:PRO:HG3	1.96	0.47
1:B:327:PHE:CD2	1:A:624:ASN:HB3	2.50	0.47
1:A:106:HIS:HB3	1:A:190:TRP:CE3	2.50	0.47
1:A:184:LEU:O	1:A:188:VAL:HG23	2.15	0.47
1:B:373:PHE:CZ	1:B:427:PRO:HG2	2.50	0.46
1:A:128:LEU:HD11	1:A:156:ARG:NH1	2.31	0.46
1:A:275:GLU:O	1:A:276:MET:C	2.58	0.46
1:B:86:PHE:HE1	1:B:184:LEU:HB2	1.80	0.46
1:B:373:PHE:HZ	1:B:427:PRO:HG2	1.80	0.46
1:B:392:HIS:HB2	1:B:413:CYS:HA	1.97	0.46
1:A:588:ARG:HA	1:A:588:ARG:HD3	1.65	0.46
1:B:622:PRO:HB2	1:A:327:PHE:CZ	2.51	0.46
1:A:54:LEU:HD21	1:A:229:TYR:HB3	1.97	0.46
1:B:144:ILE:O	1:B:145:ASP:C	2.58	0.46
1:B:367:VAL:CG1	1:B:434:PHE:HB3	2.46	0.46
1:B:8:PHE:CE2	1:B:21:LEU:HD11	2.51	0.46
1:B:430:MET:O	1:B:430:MET:HG3	2.16	0.46
1:B:473:LEU:HD12	1:B:476:THR:HG21	1.97	0.46
1:B:247:SER:C	1:B:249:ASP:N	2.74	0.46
1:A:411:LEU:HD23	1:A:426:LEU:HD12	1.98	0.46
1:A:344:ARG:HA	1:A:344:ARG:HD2	1.76	0.46
1:B:17:LEU:HD12	1:B:18:PRO:HD3	1.97	0.46
1:B:22:GLU:HG2	1:B:23:ILE:HG12	1.97	0.46
1:A:383:VAL:HG21	1:A:430:MET:HE1	1.98	0.46
1:B:410:VAL:HG12	1:B:427:PRO:HA	1.97	0.45
1:A:204:ASP:CG	1:A:205:PHE:N	2.73	0.45
1:B:187:ILE:HD13	1:B:200:VAL:HG11	1.97	0.45
1:B:585:LEU:HD22	1:B:606:GLY:O	2.16	0.45
1:A:286:GLU:HG2	1:A:287:VAL:N	2.31	0.45
1:A:417:LEU:O	1:A:418:LYS:C	2.59	0.45
1:B:86:PHE:CZ	1:B:202:LEU:HD13	2.52	0.45
1:B:63:ILE:HD11	1:B:76:PHE:HE1	1.82	0.45
1:A:187:ILE:O	1:A:190:TRP:O	2.35	0.45
1:B:54:LEU:HD21	1:B:229:TYR:CD2	2.51	0.45
1:A:63:ILE:HD11	1:A:76:PHE:CE1	2.52	0.45
1:B:183:THR:OG1	1:B:186:GLU:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLY:C	1:B:242:ILE:HG12	2.42	0.45
1:B:359:LYS:HD3	1:B:391:VAL:HG21	1.99	0.45
1:A:319:LEU:HD12	1:A:483:GLU:HG2	1.99	0.45
1:B:546:TYR:CG	1:B:547:GLU:N	2.85	0.45
1:A:148:ILE:HG23	1:A:167:LEU:HD12	1.99	0.45
1:B:269:SER:H	1:B:272:ASP:HB2	1.81	0.45
1:A:270:THR:HG21	1:A:509:LEU:O	2.17	0.44
1:A:319:LEU:HD22	1:A:540:TYR:CE1	2.51	0.44
1:A:474:ALA:O	1:A:476:THR:HG23	2.16	0.44
1:A:245:LEU:HD12	1:A:247:SER:OG	2.17	0.44
1:B:128:LEU:HD11	1:B:156:ARG:NH1	2.31	0.44
1:A:289:GLU:HB2	1:A:512:THR:H	1.81	0.44
1:B:352:ALA:HB3	1:B:428:LEU:HA	1.98	0.44
1:B:449:LEU:HD13	1:B:457:PHE:HE2	1.83	0.44
1:B:592:PHE:CD2	1:A:545:ARG:NH2	2.85	0.44
1:B:600:ASP:HB3	1:B:603:TRP:O	2.18	0.44
1:A:278:SER:O	1:A:279:LYS:C	2.59	0.44
1:A:343:LYS:NZ	1:A:441:LYS:HZ3	2.15	0.44
1:A:350:PRO:HD2	1:A:354:ASP:OD2	2.17	0.44
1:A:596:MET:HB2	1:A:596:MET:HE3	1.70	0.44
1:B:599:SER:HA	1:A:598:ASN:OD1	2.18	0.44
1:B:323:ILE:HD11	1:B:458:ASN:HB3	1.99	0.44
1:B:392:HIS:HB2	1:B:413:CYS:CB	2.48	0.44
1:A:344:ARG:HG3	1:A:345:ARG:N	2.33	0.44
1:B:378:ASP:O	1:B:379:LYS:C	2.61	0.44
1:B:548:SER:HB2	1:B:550:ALA:HB2	2.00	0.44
1:B:342:PHE:CE2	1:B:446:ILE:HB	2.53	0.44
1:A:193:PRO:HG2	1:A:196:ARG:HB2	1.99	0.44
1:B:8:PHE:HE2	1:B:21:LEU:HD11	1.83	0.43
1:B:335:PRO:HD2	1:B:532:VAL:HG22	2.00	0.43
1:B:55:LYS:HB2	1:B:232:GLN:NE2	2.33	0.43
1:B:63:ILE:HD11	1:B:76:PHE:CE1	2.53	0.43
1:B:326:ASN:N	1:B:326:ASN:HD22	2.17	0.43
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.83	0.43
1:B:351:THR:HG22	1:B:354:ASP:OD2	2.18	0.43
1:A:106:HIS:HB3	1:A:190:TRP:HE3	1.83	0.43
1:A:135:GLN:O	1:A:154:VAL:HG12	2.18	0.43
1:A:381:SER:OG	1:A:425:LEU:N	2.44	0.43
1:B:52:THR:HG23	1:B:233:GLY:HA2	2.00	0.43
1:B:284:VAL:HG23	1:B:516:VAL:HB	2.00	0.43
1:B:412:ALA:HA	1:B:424:ALA:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:HD12	1:B:504:ILE:HG23	1.81	0.43
1:A:150:VAL:HG12	1:A:165:LEU:O	2.19	0.43
1:B:333:LEU:HD21	1:B:543:MET:HE2	2.00	0.43
1:A:271:GLU:O	1:A:275:GLU:HG2	2.18	0.43
1:B:20:VAL:C	1:B:21:LEU:HD12	2.44	0.43
1:A:52:THR:HG23	1:A:233:GLY:HA2	2.00	0.43
1:A:90:ALA:HB2	1:A:176:CYS:O	2.18	0.43
1:A:271:GLU:O	1:A:274:PHE:HB3	2.18	0.43
1:A:353:TYR:O	1:A:357:ILE:HG12	2.19	0.43
1:B:20:VAL:HG12	1:B:256:THR:HG22	2.01	0.43
1:B:292:GLU:HA	1:B:298:GLN:HE22	1.84	0.43
1:B:517:SER:OG	1:B:518:ASN:N	2.52	0.43
1:B:539:GLN:O	1:B:543:MET:HG2	2.18	0.43
1:B:105:ILE:HD13	1:B:193:PRO:HB3	1.99	0.42
1:A:359:LYS:HD2	1:A:392:HIS:C	2.44	0.42
1:A:446:ILE:HD11	1:A:481:LEU:HD21	1.99	0.42
1:B:366:HIS:HE2	1:B:416:ILE:HG13	1.82	0.42
1:B:432:GLY:HA3	1:B:434:PHE:CE2	2.54	0.42
1:B:557:PRO:HG2	1:A:616:PRO:HB3	2.01	0.42
1:B:9:VAL:HA	1:B:12:LEU:HB2	2.01	0.42
1:B:297:PRO:HG3	1:B:502:TRP:CG	2.54	0.42
1:A:464:ARG:NH1	1:A:465:ASP:O	2.52	0.42
1:A:490:LEU:HG	1:A:506:VAL:HG12	2.00	0.42
1:B:371:LYS:HD2	1:B:431:GLU:HG2	2.00	0.42
1:A:359:LYS:HG2	1:A:391:VAL:HG12	2.01	0.42
1:B:103:ARG:O	1:B:194:LYS:HD3	2.19	0.42
1:A:60:ILE:HG13	1:A:226:LYS:HG3	2.01	0.42
1:B:365:LEU:N	1:B:391:VAL:HG22	2.33	0.42
1:A:22:GLU:O	1:A:23:ILE:HG22	2.20	0.42
1:B:86:PHE:CZ	1:B:184:LEU:HD12	2.55	0.42
1:A:104:THR:HG23	1:A:194:LYS:O	2.19	0.42
1:B:382:SER:OG	1:B:383:VAL:N	2.53	0.41
1:B:50:LYS:HD2	1:B:51:ILE:H	1.85	0.41
1:A:485:ILE:HD13	1:A:543:MET:HE2	2.02	0.41
1:A:344:ARG:HH22	1:A:347:ARG:NE	2.18	0.41
1:A:585:LEU:HD22	1:A:606:GLY:O	2.20	0.41
1:B:245:LEU:HD23	1:B:246:PRO:O	2.21	0.41
1:B:596:MET:HE2	1:B:606:GLY:CA	2.49	0.41
1:A:187:ILE:HA	1:A:191:LYS:HB2	2.03	0.41
1:A:609:HIS:HB3	1:A:610:GLY:H	1.59	0.41
1:A:92:LYS:HD3	1:A:92:LYS:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:MET:HB2	1:A:276:MET:HE2	1.80	0.41
1:A:277:THR:O	1:A:278:SER:C	2.63	0.41
1:B:19:ARG:HD3	1:B:254:ASP:OD2	2.21	0.41
1:B:99:GLU:HA	1:B:167:LEU:HD22	2.03	0.41
1:B:306:THR:HG22	1:B:495:PHE:HB2	2.03	0.41
1:B:410:VAL:CG2	1:B:425:LEU:HD12	2.51	0.41
1:A:273:LEU:HA	1:A:276:MET:HE3	2.03	0.41
1:A:274:PHE:O	1:A:275:GLU:C	2.64	0.41
1:A:445:PRO:HG2	1:A:448:GLU:HG2	2.02	0.41
1:A:495:PHE:HD1	1:A:495:PHE:HA	1.70	0.41
1:A:285:THR:HB	1:A:513:VAL:HB	2.03	0.41
1:A:379:LYS:HG3	1:A:425:LEU:HD12	2.03	0.41
1:B:473:LEU:HD11	1:B:479:LEU:HD11	2.03	0.40
1:B:598:ASN:HA	1:B:604:TRP:CD1	2.56	0.40
1:A:499:THR:HB	1:A:526:PHE:HB2	2.03	0.40
1:A:473:LEU:HA	1:A:476:THR:HG21	2.03	0.40
1:B:227:PRO:HG2	1:B:229:TYR:CZ	2.56	0.40
1:B:351:THR:HG23	1:B:354:ASP:H	1.87	0.40
1:A:137:MET:O	1:A:152:CYS:HA	2.21	0.40
1:A:255:ILE:HG13	1:A:258:SER:HB2	2.02	0.40
1:A:54:LEU:HD21	1:A:229:TYR:CD1	2.56	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	505/648 (78%)	456 (90%)	45 (9%)	4 (1%)	16	42
1	B	493/648 (76%)	450 (91%)	39 (8%)	4 (1%)	16	42
All	All	998/1296 (77%)	906 (91%)	84 (8%)	8 (1%)	16	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	PRO
1	A	433	GLY
1	B	478	GLY
1	A	282	PRO
1	B	282	PRO
1	A	498	PRO
1	B	297	PRO
1	B	246	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	486/588 (83%)	468 (96%)	18 (4%)	30	57
1	B	476/588 (81%)	457 (96%)	19 (4%)	28	56
All	All	962/1176 (82%)	925 (96%)	37 (4%)	29	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	LEU
1	B	145	ASP
1	B	172	GLU
1	B	177	GLU
1	B	246	PRO
1	B	248	LEU
1	B	277	THR
1	B	283	ILE
1	B	294	ASN
1	B	378	ASP
1	B	379	LYS
1	B	381	SER
1	B	392	HIS
1	B	393	GLN
1	B	463	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	497	ASN
1	B	544	ARG
1	B	546	TYR
1	B	548	SER
1	A	19	ARG
1	A	20	VAL
1	A	21	LEU
1	A	22	GLU
1	A	23	ILE
1	A	168	SER
1	A	187	ILE
1	A	192	ILE
1	A	275	GLU
1	A	278	SER
1	A	279	LYS
1	A	280	GLU
1	A	282	PRO
1	A	283	ILE
1	A	327	PHE
1	A	329	LYS
1	A	417	LEU
1	A	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	GLN
1	B	298	GLN
1	B	326	ASN
1	B	560	HIS
1	A	326	ASN
1	A	392	HIS
1	A	560	HIS
1	A	594	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	527/648 (81%)	0.30	9 (1%) 69 46	30, 94, 136, 168	0
1	B	521/648 (80%)	0.26	5 (0%) 79 59	62, 96, 141, 159	0
All	All	1048/1296 (80%)	0.28	14 (1%) 75 53	30, 94, 140, 168	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	GLU	4.2
1	A	378	ASP	3.5
1	B	140	SER	3.4
1	A	279	LYS	3.4
1	B	457	PHE	2.9
1	B	375	SER	2.4
1	A	161	HIS	2.3
1	A	366	HIS	2.3
1	A	568	PRO	2.2
1	A	245	LEU	2.2
1	B	14	LEU	2.2
1	B	431	GLU	2.2
1	A	21	LEU	2.1
1	A	407	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.