



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:40 AM EDT

PDB ID : 6QDM / pdb_00006qdm
Title : Molecular features of the UNC-45 chaperone critical for binding and folding muscle myosin
Authors : Meinhart, A.; Clausen, T.; Hellerschmied, D.
Deposited on : 2019-01-02
Resolution : 3.80 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

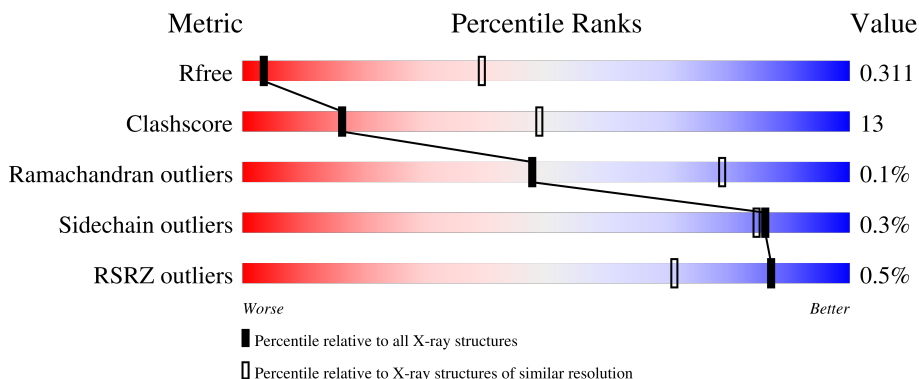
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	963	 58% 23% 19%
1	B	963	 55% 21% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11813 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 UNC-45,UNC-45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	776	Total 6035	C 3830	N 1028	O 1134	S 43	0	0	0
1	B	739	Total 5778	C 3670	N 981	O 1085	S 42	0	0	0

V908	L799	L679	V589	GLU	V349	D230	LEU	ASP	MET
L909	L802	R680	Y590	ARG	A350	F231	GLN	ASP	VAL
K914	F806	E686	T591	ALA	S951	D232	ARG	PHE	ALA
L915	F805	T689	L592	ILE	D352	G233	LEU	GLY	ARG
UNK	K807	L693	A593	M477	I353	P234	VAL	GLY	VAL
UNK	L820	T696	T594	L478	K285	K285	ALA	GLN	GLN
UNK	Y826	K697	M601	K479	C357	C241	ASN	THR	ALA
UNK	V630	T699	E604	I482	E358	R242	ASN	ALA	ALA
UNK	V630	S700	K605	P483	Y369	P360	ASP	GLU	GLU
UNK	R634	K704	P80	R486	V361	L243	ASP	THR	ILE
UNK	L835	I705	LYS	E863	S362	Q261	ASP	LYS	ARG
UNK	L836	G706	VAL	E364	N265	N265	LEU	GLU	GLU
UNK	S836	K706	ASP	H368	M270	M270	GLU	GLY	ASN
UNK	R837	A707	GLU	H368	D271	D271	ASP	ALA	ALA
UNK	A838	G708	MET	V369	R272	R272	ALA	VAL	VAL
UNK	A841	I711	VAL	A370	E284	E284	LYS	ASP	LYS
UNK	I845	L714	LYS	I371	A285	A285	VAL	VAL	ASP
UNK	E848	G715	LEU	K385	N286	N286	GLN	GLN	GLN
UNK	D849	A716	ALA	D394	K287	K287	LEU	TYR	TYR
UNK	E850	V732	ALA	R898	I288	I288	PHE	ILE	ILE
UNK	C853	P735	GLY	I401	W289	W289	ARG	LYS	LYS
UNK	R855	H741	GLY	C404	I290	I290	ALA	ASP	ASP
UNK	I856	D742	GLY	K416	R292	R292	LEU	LEU	LEU
UNK	M857	D743	ASP	F420	R311	R311	GLY	GLY	GLY
UNK	A858	V762	ILE	L425	E312	E312	ASN	ASN	ASN
UNK	E859	I766	SER	L436	L319	L319	LEU	LEU	LEU
UNK	C853	R767	THR	T437	R320	R320	GLY	THR	THR
UNK	R863	I770	THR	M438	N321	N321	PRO	THR	THR
UNK	P864	L771	LYS	D439	I322	I322	ALA	ALA	ALA
UNK	F867	I776	ALA	Q440	M323	M323	ALA	ALA	ALA
UNK	I870	P777	ALA	L441	D326	D326	LYS	LYS	LYS
UNK	H873	E780	LYS	T442	G327	G327	ALA	ALA	ALA
UNK	D874	E781	GLU	P443	G328	G328	LEU	LEU	LEU
UNK	D875	F782	GLU	E447	I329	I329	ARG	ARG	ARG
UNK	A876	W783	VAL	D453	V335	V335	ALA	ALA	ALA
UNK	T878	F784	VAL	I459	V336	V336	LEU	LEU	LEU
UNK	T879	M785	VAL	E462	R341	R341	LEU	LEU	LEU
UNK	R880	H788	VAL	A466	L343	L343	PRO	PRO	PRO
UNK	R881	L791	VAL	T467	I344	I344	ALA	ALA	ALA
UNK	S892	R792	VAL	V468	A345	A345	ARG	ARG	ARG
UNK	L896	A793	VAL	S469	L346	L346	LEU	LEU	LEU
UNK	V905	A796	VAL	K470	S469	S469	LYS	LYS	LYS
UNK	F906	R907	VAL	HIS	L347	L347	GLU	GLU	GLU
UNK	R907				D348	D348	VAL	VAL	VAL

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.39Å 97.61Å 148.88Å 90.00° 93.41° 90.00°	Depositor
Resolution (Å)	48.80 – 3.80 48.80 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.80-3.80) 89.0 (48.80-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 3.77Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???), CNS	Depositor
R, R_{free}	0.280 , 0.310 0.283 , 0.311	Depositor DCC
R_{free} test set	1137 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	173.5	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 159.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11813	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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 i

5.1 Standard geometry i

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	0.65	1/6058 (0.0%)	0.91	0/8178
1	B	0.62	0/5863	0.89	3/7912 (0.0%)
All	All	0.63	1/11921 (0.0%)	0.90	3/16090 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	648	VAL	CA-CB	5.52	1.57	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	MET	N-CA-C	-5.92	105.91	113.01
1	B	438	ASN	CA-C-N	5.68	132.63	122.06
1	B	438	ASN	C-N-CA	5.68	132.63	122.06

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	6035	0	6128	156	4
1	B	5778	0	5926	156	2
All	All	11813	0	12054	310	4

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 13.

All (310) 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:B:441:LEU:HD23	1:B:477:MET:SD	1.82	1.19
1:A:229:HIS:O	1:A:230:ASP:OD1	1.85	0.95
1:B:441:LEU:HG	1:B:477:MET:HE1	1.59	0.83
1:B:229:HIS:O	1:B:230:ASP:CG	2.21	0.83
1:B:551:CYS:SG	1:B:580:LEU:HD22	2.19	0.83
1:B:742:PRO:HG3	1:B:782:PHE:CE2	2.14	0.83
1:A:850:GLU:HG2	1:A:892:SER:HB2	1.61	0.82
1:B:319:LEU:HD11	1:B:371:ILE:HG22	1.62	0.81
1:B:551:CYS:SG	1:B:580:LEU:CD2	2.69	0.81
1:B:186:ALA:O	1:B:189:PRO:HD2	1.81	0.79
1:B:229:HIS:O	1:B:230:ASP:OD1	2.00	0.79
1:B:732:VAL:O	1:B:735:PRO:HD2	1.84	0.78
1:A:548:ARG:HD3	1:A:587:LEU:HG	1.65	0.77
1:B:441:LEU:CD2	1:B:477:MET:SD	2.70	0.77
1:A:483:PRO:HA	1:A:486:ARG:HD2	1.66	0.76
1:B:156:ASP:HB3	1:B:159:GLN:HG2	1.68	0.75
1:B:150:PHE:CD1	1:B:190:PHE:HB3	2.21	0.75
1:B:441:LEU:HG	1:B:477:MET:CE	2.17	0.75
1:A:229:HIS:O	1:A:230:ASP:CG	2.31	0.74
1:A:674:ALA:O	1:A:680:ARG:NH2	2.20	0.74
1:A:589:VAL:HG22	1:A:654:VAL:HB	1.70	0.74
1:A:732:VAL:O	1:A:735:PRO:HD2	1.88	0.73
1:A:271:ASP:HB2	1:A:276:MET:HE2	1.72	0.72
1:A:150:PHE:CG	1:A:190:PHE:HB3	2.25	0.71
1:B:530:LYS:NZ	1:B:533:LYS:HD3	2.05	0.71
1:B:467:THR:HB	1:B:478:LEU:HD21	1.72	0.71
1:B:788:HIS:HB2	1:B:834:ARG:HH22	1.53	0.71
1:A:475:ILE:HA	1:A:478:LEU:HB2	1.73	0.70
1:A:907:ARG:HD3	1:A:908:VAL:HG13	1.73	0.70
1:A:146:GLU:OE2	1:A:151:ARG:NH2	2.26	0.69
1:A:602:ALA:HA	1:A:605:LYS:HB2	1.76	0.68
1:A:150:PHE:CD1	1:A:190:PHE:HB3	2.28	0.68
1:A:785:MET:O	1:A:792:ARG:NH2	2.26	0.68
1:B:489:TYR:O	1:B:497:LYS:NZ	2.27	0.67
1:B:857:MET:HG3	1:B:896:LEU:HD22	1.77	0.66
1:B:272:ARG:NH2	1:B:326:ASP:OD2	2.29	0.66
1:A:501:LEU:HD21	1:A:532:CYS:SG	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ILE:HA	1:B:404:CYS:SG	2.37	0.64
1:B:799:LEU:HD23	1:B:802:LEU:HD12	1.80	0.63
1:B:586:ALA:HB1	1:B:657:THR:HG23	1.80	0.63
1:A:640:ARG:NH1	1:A:678:ASP:OD2	2.25	0.63
1:B:530:LYS:HZ1	1:B:533:LYS:HD3	1.64	0.63
1:B:425:LEU:HD13	1:B:466:ALA:C	2.23	0.63
1:B:742:PRO:HG3	1:B:782:PHE:CZ	2.33	0.62
1:B:877:GLU:OE1	1:B:880:ARG:NH1	2.26	0.62
1:B:680:ARG:HH12	1:B:716:ALA:HB3	1.65	0.62
1:A:602:ALA:HB1	1:A:668:ARG:HB3	1.82	0.61
1:B:788:HIS:HB2	1:B:834:ARG:NH2	2.15	0.61
1:B:319:LEU:HD11	1:B:371:ILE:CG2	2.31	0.61
1:A:483:PRO:O	1:A:486:ARG:HB2	2.01	0.61
1:A:830:VAL:HG21	1:A:873:HIS:NE2	2.16	0.61
1:B:436:ILE:HG23	1:B:477:MET:SD	2.40	0.61
1:B:776:ILE:HB	1:B:777:PRO:HD3	1.83	0.61
1:A:270:MET:HE1	1:A:328:GLY:HA2	1.82	0.61
1:A:907:ARG:HG2	1:B:495:THR:HG21	1.82	0.60
1:A:183:ASN:HB3	1:A:186:ALA:HB3	1.82	0.60
1:A:230:ASP:HB2	1:A:236:SER:HB2	1.82	0.60
1:B:323:MET:SD	1:B:323:MET:N	2.74	0.60
1:A:805:PHE:HE2	1:A:807:LYS:HB3	1.66	0.60
1:B:762:VAL:HG13	1:B:766:ILE:HG13	1.82	0.60
1:A:914:LYS:NZ	1:B:453:ASP:OD2	2.33	0.60
1:B:589:VAL:HG22	1:B:654:VAL:HB	1.83	0.60
1:A:427:GLY:O	1:A:429:VAL:HG23	2.01	0.60
1:B:186:ALA:C	1:B:189:PRO:HD2	2.27	0.59
1:A:876:ALA:HA	1:A:879:GLN:HG2	1.85	0.59
1:A:629:LYS:HA	1:A:634:TYR:HD2	1.68	0.59
1:A:384:THR:O	1:A:388:ILE:HG12	2.02	0.59
1:A:425:LEU:HD13	1:A:466:ALA:O	2.02	0.58
1:B:311:ARG:NH1	1:B:360:PRO:O	2.35	0.58
1:B:468:VAL:HG22	1:B:478:LEU:HD13	1.84	0.58
1:B:649:PRO:HA	1:B:652:VAL:HG22	1.85	0.58
1:A:533:LYS:NZ	1:A:566:TRP:CZ2	2.69	0.58
1:A:789:GLU:HA	1:A:834:ARG:NH2	2.17	0.57
1:A:533:LYS:HZ2	1:A:566:TRP:HZ2	1.50	0.57
1:A:286:ASN:HB2	1:A:289:TRP:HD1	1.68	0.57
1:B:150:PHE:CE1	1:B:190:PHE:HB3	2.40	0.57
1:A:451:SER:O	1:A:457:GLN:NE2	2.38	0.57
1:B:150:PHE:CG	1:B:190:PHE:HB3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:OD2	1:A:234:PRO:HD2	2.05	0.57
1:A:876:ALA:C	1:A:879:GLN:HG2	2.30	0.57
1:A:164:LEU:HD11	1:A:204:VAL:HG13	1.85	0.56
1:B:425:LEU:HD13	1:B:467:THR:N	2.20	0.56
1:B:792:ARG:H	1:B:834:ARG:NH1	2.02	0.56
1:A:467:THR:HG22	1:A:478:LEU:HD11	1.87	0.56
1:B:855:ARG:NE	1:B:859:GLU:OE2	2.34	0.56
1:B:741:HIS:HB3	1:B:743:ASP:OD1	2.05	0.56
1:A:287:LYS:HG3	1:A:333:TRP:CH2	2.41	0.56
1:A:242:ARG:NH2	1:A:303:ASP:OD2	2.39	0.56
1:A:498:VAL:HG21	1:A:546:ILE:HG23	1.88	0.55
1:A:805:PHE:CE2	1:A:807:LYS:HB3	2.41	0.55
1:A:147:LYS:HE3	1:A:151:ARG:HD2	1.88	0.55
1:A:287:LYS:HG3	1:A:333:TRP:HH2	1.72	0.55
1:B:179:THR:OG1	1:B:221:ARG:NH2	2.40	0.55
1:A:876:ALA:HA	1:A:879:GLN:CD	2.31	0.55
1:B:788:HIS:ND1	1:B:791:LEU:HD12	2.22	0.55
1:A:663:LEU:HD23	1:A:666:ILE:HD12	1.87	0.55
1:A:599:LEU:HD13	1:A:642:LEU:HD11	1.89	0.54
1:A:192:LEU:HD23	1:A:195:ILE:HD12	1.89	0.54
1:A:533:LYS:NZ	1:A:566:TRP:HZ2	2.05	0.54
1:A:562:ASP:OD1	1:A:629:LYS:NZ	2.31	0.54
1:B:441:LEU:CG	1:B:477:MET:CE	2.86	0.54
1:A:602:ALA:O	1:A:668:ARG:HD3	2.07	0.54
1:A:237:VAL:HG12	1:A:296:GLU:HG3	1.89	0.53
1:A:876:ALA:O	1:A:879:GLN:HG2	2.07	0.53
1:A:279:ASP:HB3	1:A:282:VAL:HG22	1.90	0.53
1:B:270:MET:HE1	1:B:328:GLY:HA2	1.89	0.53
1:A:338:VAL:O	1:A:392:LYS:NZ	2.42	0.53
1:A:485:LEU:HD21	1:A:500:ALA:O	2.09	0.53
1:A:762:VAL:HG13	1:A:766:ILE:HG13	1.91	0.53
1:B:287:LYS:HA	1:B:290:ILE:HD12	1.91	0.53
1:A:767:ARG:HA	1:A:770:ILE:HD12	1.91	0.53
1:B:341:ARG:H	1:B:341:ARG:HD2	1.74	0.53
1:B:850:GLU:HG3	1:B:892:SER:HB2	1.91	0.52
1:A:890:MET:HB3	1:A:897:CYS:SG	2.50	0.52
1:A:354:PRO:HG3	1:A:362:SER:HA	1.91	0.52
1:B:776:ILE:O	1:B:780:GLU:HG3	2.10	0.52
1:B:171:CYS:HB2	1:B:178:ALA:HB2	1.92	0.52
1:B:230:ASP:HB2	1:B:236:SER:HB2	1.92	0.52
1:B:311:ARG:HH22	1:B:360:PRO:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ALA:HB2	1:B:369:VAL:HG11	1.92	0.51
1:B:482:ILE:HB	1:B:483:PRO:HD3	1.92	0.51
1:A:164:LEU:HB3	1:A:207:THR:HG21	1.92	0.51
1:B:232:ASP:OD2	1:B:234:PRO:HD2	2.10	0.51
1:B:489:TYR:HE1	1:B:501:LEU:HD13	1.75	0.51
1:B:627:HIS:CD2	1:B:629:LYS:H	2.29	0.51
1:B:591:THR:OG1	1:B:592:LEU:N	2.42	0.51
1:A:855:ARG:NH2	1:A:859:GLU:OE1	2.44	0.51
1:A:736:LEU:HD11	1:A:756:LEU:HD21	1.93	0.50
1:B:208:ALA:O	1:B:211:ILE:HB	2.10	0.50
1:B:526:ILE:O	1:B:530:LYS:HG2	2.12	0.50
1:B:627:HIS:CD2	1:B:629:LYS:HB2	2.46	0.50
1:B:151:ARG:HH21	1:B:190:PHE:HZ	1.60	0.50
1:B:660:LYS:HB3	1:B:700:SER:HB3	1.93	0.50
1:B:826:TYR:HB3	1:B:835:LEU:HD11	1.94	0.50
1:B:138:LEU:HD11	1:B:180:GLY:HA3	1.93	0.50
1:B:633:GLU:OE1	1:B:633:GLU:N	2.42	0.50
1:A:888:ASN:N	1:A:888:ASN:OD1	2.42	0.49
1:B:785:MET:O	1:B:834:ARG:NH2	2.45	0.49
1:A:746:GLY:C	1:A:748:ALA:H	2.20	0.49
1:B:353:ILE:HG13	1:B:356:LEU:H	1.77	0.49
1:A:316:ASP:OD1	1:A:368:HIS:ND1	2.44	0.49
1:A:605:LYS:HZ2	1:A:672:ALA:HB2	1.78	0.49
1:A:143:THR:HG23	1:A:147:LYS:HZ3	1.77	0.49
1:B:338:VAL:HG13	1:B:343:LEU:HD22	1.94	0.49
1:B:437:THR:O	1:B:439:ASP:OD1	2.31	0.49
1:B:793:ALA:N	1:B:834:ARG:HD2	2.28	0.49
1:B:161:MET:HE2	1:B:204:VAL:HG22	1.95	0.48
1:A:857:MET:HG3	1:A:896:LEU:HD22	1.95	0.48
1:A:873:HIS:ND1	1:A:875:ASP:O	2.36	0.48
1:A:876:ALA:HA	1:A:879:GLN:CG	2.42	0.48
1:A:405:THR:O	1:A:414:ARG:NH1	2.45	0.48
1:A:876:ALA:CA	1:A:879:GLN:HG2	2.43	0.48
1:B:306:VAL:O	1:B:311:ARG:NH2	2.46	0.48
1:B:767:ARG:HA	1:B:770:ILE:HD12	1.96	0.48
1:A:530:LYS:O	1:A:533:LYS:HB3	2.13	0.48
1:A:506:LYS:HA	1:A:556:TYR:HB3	1.95	0.48
1:B:177:GLY:O	1:B:181:VAL:HG23	2.13	0.48
1:A:736:LEU:HA	1:A:739:LEU:HD13	1.95	0.48
1:A:324:HIS:HA	1:A:328:GLY:H	1.79	0.48
1:B:443:PRO:O	1:B:447:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLU:O	1:A:680:ARG:HG2	2.14	0.47
1:B:206:VAL:HG12	1:B:210:ARG:NH1	2.29	0.47
1:B:161:MET:HE1	1:B:203:GLU:C	2.39	0.47
1:A:629:LYS:HA	1:A:634:TYR:CD2	2.49	0.47
1:B:836:SER:HB2	1:B:878:THR:HG21	1.96	0.47
1:A:482:ILE:HB	1:A:483:PRO:HD3	1.96	0.47
1:B:697:LYS:O	1:B:704:LYS:NZ	2.46	0.47
1:B:551:CYS:SG	1:B:580:LEU:HD21	2.54	0.47
1:A:793:ALA:HB2	1:A:834:ARG:HH11	1.79	0.47
1:B:394:ASP:O	1:B:398:ASN:ND2	2.47	0.47
1:B:530:LYS:HZ2	1:B:533:LYS:HD3	1.77	0.47
1:B:261:GLN:OE1	1:B:321:ASN:ND2	2.38	0.47
1:B:601:ASN:OD1	1:B:638:ARG:NH1	2.47	0.47
1:B:668:ARG:HG2	1:B:706:LYS:HE3	1.96	0.47
1:B:870:ILE:O	1:B:873:HIS:HB2	2.15	0.47
1:B:242:ARG:HD3	1:B:300:MET:HE3	1.95	0.47
1:A:586:ALA:HB1	1:A:657:THR:HG23	1.97	0.47
1:A:609:ASP:O	1:A:613:VAL:HG23	2.14	0.47
1:B:857:MET:CG	1:B:896:LEU:HD22	2.44	0.47
1:B:634:TYR:O	1:B:638:ARG:HG3	2.15	0.46
1:B:146:GLU:OE2	1:B:151:ARG:NH2	2.48	0.46
1:B:648:VAL:HB	1:B:649:PRO:HD3	1.98	0.46
1:A:901:VAL:HG22	1:A:906:PHE:CE1	2.50	0.46
1:A:677:GLU:HA	1:A:680:ARG:NE	2.30	0.46
1:A:148:LEU:HD12	1:A:153:GLU:OE1	2.16	0.46
1:B:863:TRP:CD2	1:B:864:PRO:HD3	2.50	0.46
1:B:242:ARG:HE	1:B:300:MET:HG2	1.80	0.46
1:A:230:ASP:OD2	1:A:235:LYS:C	2.59	0.46
1:A:505:CYS:HB3	1:A:553:GLY:O	2.16	0.45
1:A:805:PHE:HD2	1:A:808:PHE:H	1.62	0.45
1:B:265:ASN:ND2	1:B:270:MET:O	2.45	0.45
1:B:398:ASN:HA	1:B:401:ILE:HG22	1.99	0.45
1:A:833:GLU:O	1:A:837:ARG:HG3	2.17	0.45
1:B:820:LEU:HA	1:B:820:LEU:HD23	1.72	0.45
1:B:227:ALA:HB2	1:B:289:TRP:CH2	2.52	0.45
1:A:401:ILE:HA	1:A:404:CYS:SG	2.56	0.45
1:A:427:GLY:O	1:A:429:VAL:N	2.49	0.45
1:B:483:PRO:O	1:B:486:ARG:HB2	2.17	0.45
1:B:783:TRP:HA	1:B:792:ARG:HG3	1.98	0.45
1:B:792:ARG:HB3	1:B:834:ARG:CZ	2.47	0.45
1:B:286:ASN:HB2	1:B:289:TRP:HD1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:SER:HB2	1:A:416:LYS:HB3	1.99	0.45
1:A:443:PRO:O	1:A:447:GLU:HG3	2.17	0.45
1:B:312:GLU:OE2	1:B:362:SER:OG	2.34	0.45
1:A:603:PHE:HA	1:A:668:ARG:NH1	2.32	0.45
1:A:853:CYS:SG	1:A:889:ILE:HG12	2.57	0.45
1:B:627:HIS:NE2	1:B:629:LYS:HB2	2.32	0.45
1:A:347:LEU:HD22	1:A:420:PHE:HE1	1.82	0.45
1:A:347:LEU:HD22	1:A:420:PHE:CE1	2.52	0.45
1:A:742:PRO:HG3	1:A:782:PHE:CE2	2.52	0.45
1:A:708:GLY:HA2	1:A:711:ILE:HD12	1.98	0.44
1:B:853:CYS:HA	1:B:856:ILE:HD12	1.99	0.44
1:A:709:HIS:NE2	1:A:713:LYS:HE3	2.32	0.44
1:B:188:VAL:HG13	1:B:189:PRO:HD3	1.99	0.44
1:B:284:GLU:OE1	1:B:287:LYS:HD2	2.17	0.44
1:B:805:PHE:CE2	1:B:807:LYS:HB3	2.53	0.44
1:A:320:LYS:HD3	1:A:658:GLU:OE2	2.17	0.44
1:A:759:LEU:O	1:A:762:VAL:HG12	2.17	0.44
1:A:789:GLU:HA	1:A:834:ARG:CZ	2.48	0.44
1:A:820:LEU:HA	1:A:820:LEU:HD23	1.68	0.44
1:A:352:GLN:OE1	1:A:357:CYS:HA	2.18	0.44
1:B:873:HIS:HE1	1:B:875:ASP:HB3	1.83	0.44
1:A:743:ASP:OD1	1:A:743:ASP:N	2.50	0.44
1:A:873:HIS:HB3	1:A:879:GLN:OE1	2.18	0.44
1:B:906:PHE:HA	1:B:909:LEU:HD12	1.98	0.44
1:A:197:ASP:OD1	1:A:199:SER:N	2.41	0.43
1:A:828:ALA:HB2	1:A:866:VAL:HG13	1.99	0.43
1:B:489:TYR:CE1	1:B:501:LEU:HD13	2.52	0.43
1:B:321:ASN:O	1:B:329:ILE:HG12	2.17	0.43
1:B:506:LYS:HA	1:B:556:TYR:HB3	2.00	0.43
1:A:876:ALA:HA	1:A:879:GLN:NE2	2.33	0.43
1:A:479:LYS:O	1:A:482:ILE:HD12	2.19	0.43
1:B:358:GLU:N	1:B:358:GLU:OE1	2.51	0.43
1:B:643:VAL:HG21	1:B:679:LEU:HD13	2.01	0.43
1:B:826:TYR:CG	1:B:835:LEU:HD21	2.54	0.43
1:B:552:GLU:HA	1:B:591:THR:HB	2.01	0.43
1:A:213:ASP:OD1	1:A:214:GLU:N	2.52	0.43
1:A:330:PRO:O	1:A:333:TRP:HD1	2.02	0.43
1:B:345:ALA:O	1:B:349:VAL:HG23	2.19	0.43
1:B:347:LEU:HD22	1:B:420:PHE:HE1	1.84	0.43
1:B:229:HIS:HB2	1:B:236:SER:OG	2.19	0.43
1:A:649:PRO:HA	1:A:652:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:PHE:HB2	1:B:905:VAL:HG21	2.01	0.43
1:A:870:ILE:HD11	1:A:886:ILE:HD11	2.01	0.42
1:B:364:GLU:HG2	1:B:368:HIS:CD2	2.54	0.42
1:A:467:THR:CG2	1:A:478:LEU:HD11	2.49	0.42
1:A:643:VAL:HG11	1:A:679:LEU:HB3	2.01	0.42
1:A:780:GLU:HB3	1:A:784:PHE:CZ	2.54	0.42
1:B:233:GLY:HA3	1:B:292:ARG:NH1	2.35	0.42
1:B:792:ARG:HD2	1:B:835:LEU:HD22	2.01	0.42
1:B:845:ILE:O	1:B:848:GLU:HG2	2.19	0.42
1:A:286:ASN:HB2	1:A:289:TRP:CD1	2.52	0.42
1:A:716:ALA:O	1:A:754:LEU:HG	2.19	0.42
1:B:226:LEU:O	1:B:236:SER:OG	2.27	0.42
1:A:213:ASP:HA	1:A:216:ILE:HG12	2.00	0.42
1:A:590:TYR:HA	1:A:662:ALA:HB2	2.01	0.42
1:A:762:VAL:CG1	1:A:766:ILE:HG13	2.48	0.42
1:A:574:LEU:HD21	1:A:642:LEU:HD23	2.01	0.42
1:B:604:GLU:OE1	1:B:604:GLU:N	2.42	0.42
1:A:218:ASN:ND2	1:A:221:ARG:HG3	2.34	0.42
1:A:366:ARG:NH1	1:A:419:CYS:HB3	2.35	0.42
1:B:708:GLY:HA2	1:B:711:ILE:HD12	2.01	0.42
1:A:142:VAL:O	1:A:146:GLU:HB2	2.20	0.42
1:A:358:GLU:OE2	1:A:416:LYS:NZ	2.30	0.42
1:A:446:LEU:HD23	1:A:446:LEU:HA	1.81	0.42
1:A:834:ARG:HG3	1:A:835:LEU:N	2.35	0.42
1:B:693:LEU:O	1:B:696:THR:HG22	2.20	0.42
1:B:796:ALA:HB1	1:B:838:ALA:HB2	2.01	0.42
1:A:284:GLU:OE1	1:A:287:LYS:HD2	2.19	0.41
1:A:353:ILE:HG23	1:A:419:CYS:SG	2.60	0.41
1:A:398:ASN:HA	1:A:401:ILE:HG22	2.01	0.41
1:A:814:ALA:HA	1:A:815:PRO:HD3	1.88	0.41
1:A:873:HIS:HE1	1:A:875:ASP:HB3	1.84	0.41
1:B:841:ALA:CB	1:B:881:ARG:HH11	2.32	0.41
1:A:865:GLU:O	1:A:868:LYS:HG2	2.21	0.41
1:B:555:SER:HB2	1:B:594:THR:HB	2.01	0.41
1:B:689:THR:HG22	1:B:714:LEU:HD13	2.02	0.41
1:B:771:LEU:HD13	1:B:805:PHE:HE2	1.84	0.41
1:B:648:VAL:HB	1:B:686:GLU:OE1	2.21	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.91	0.41
1:A:660:LYS:HB3	1:A:700:SER:HB3	2.02	0.41
1:A:627:HIS:CG	1:A:628:PRO:HD2	2.55	0.41
1:A:792:ARG:NE	1:A:835:LEU:HD22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:CD2	1:B:477:MET:CE	2.98	0.41
1:B:592:LEU:HA	1:B:592:LEU:HD12	1.88	0.41
1:B:762:VAL:CG1	1:B:766:ILE:HG13	2.50	0.41
1:B:830:VAL:HG21	1:B:873:HIS:CE1	2.55	0.41
1:A:853:CYS:SG	1:A:889:ILE:HA	2.61	0.41
1:B:352:GLN:HE22	1:B:416:LYS:HE2	1.86	0.41
1:A:470:LYS:O	1:A:470:LYS:HG2	2.20	0.41
1:A:692:CYS:HA	1:A:695:LEU:HD12	2.02	0.41
1:B:459:ILE:HA	1:B:462:GLU:HG2	2.01	0.41
1:B:548:ARG:NH2	1:B:549:TYR:OH	2.53	0.41
1:B:234:PRO:HG3	1:B:292:ARG:NE	2.36	0.41
1:B:242:ARG:HE	1:B:300:MET:CG	2.34	0.41
1:B:439:ASP:OD1	1:B:439:ASP:N	2.54	0.41
1:B:627:HIS:ND1	1:B:628:PRO:HD2	2.35	0.41
1:A:884:MET:HE3	1:A:884:MET:HB2	2.00	0.40
1:B:627:HIS:HE2	1:B:629:LYS:HB2	1.86	0.40
1:A:366:ARG:HH11	1:A:419:CYS:HB3	1.86	0.40
1:A:707:ALA:O	1:A:711:ILE:HG13	2.21	0.40
1:A:225:PHE:O	1:A:228:MET:HG2	2.22	0.40
1:A:415:ILE:HD11	1:A:456:MET:HG2	2.03	0.40
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.86	0.40
1:A:483:PRO:HA	1:A:486:ARG:HB2	2.02	0.40
1:A:329:ILE:HG22	1:A:333:TRP:CG	2.56	0.40
1:A:597:ALA:O	1:A:602:ALA:N	2.48	0.40
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.86	0.40
1:B:335:TRP:CD2	1:B:385:LYS:HE2	2.57	0.40
1:B:675:GLU:HB3	1:B:676:TYR:CE2	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLU:CG	1:A:472:GLU:CG[2_656]	1.82	0.38
1:A:355:GLU:CG	1:B:907:ARG:NH1[1_556]	1.86	0.34
1:A:453:ASP:OD2	1:B:914:LYS:NZ[1_556]	2.11	0.09
1:A:533:LYS:CE	1:A:810:GLU:OE1[4_546]	2.15	0.05

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	756/963 (78%)	726 (96%)	29 (4%)	1 (0%)	48	79
1	B	731/963 (76%)	710 (97%)	20 (3%)	1 (0%)	48	79
All	All	1487/1926 (77%)	1436 (97%)	49 (3%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASP
1	A	606	PRO

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	652/775 (84%)	651 (100%)	1 (0%)	87	87
1	B	631/775 (81%)	628 (100%)	3 (0%)	81	81
All	All	1283/1550 (83%)	1279 (100%)	4 (0%)	86	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	VAL
1	B	188	VAL
1	B	439	ASP
1	B	479	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	440	GLN
1	A	457	GLN
1	A	598	ASN
1	B	165	ASN
1	B	166	ASN
1	B	374	GLN
1	B	398	ASN
1	B	438	ASN
1	B	598	ASN
1	B	627	HIS
1	B	661	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	915:LEU	C	926:UNK	N	7.00

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	762/963 (79%)	-0.54	4 (0%) 87 71	133, 190, 238, 297	0
1	B	739/963 (76%)	-0.57	3 (0%) 88 74	142, 205, 248, 336	0
All	All	1501/1926 (77%)	-0.55	7 (0%) 87 71	133, 197, 246, 336	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	ASN	2.8
1	A	858	ASP	2.6
1	A	693	LEU	2.5
1	A	241	CYS	2.4
1	B	462	GLU	2.2
1	B	241	CYS	2.1
1	A	347	LEU	2.1

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.