



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:19 PM UTC

PDB ID : 6HEL / pdb_00006hel
Title : Structure of human USP25
Authors : Gersch, M.; Komander, D.
Deposited on : 2018-08-20
Resolution : 2.94 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)	:	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

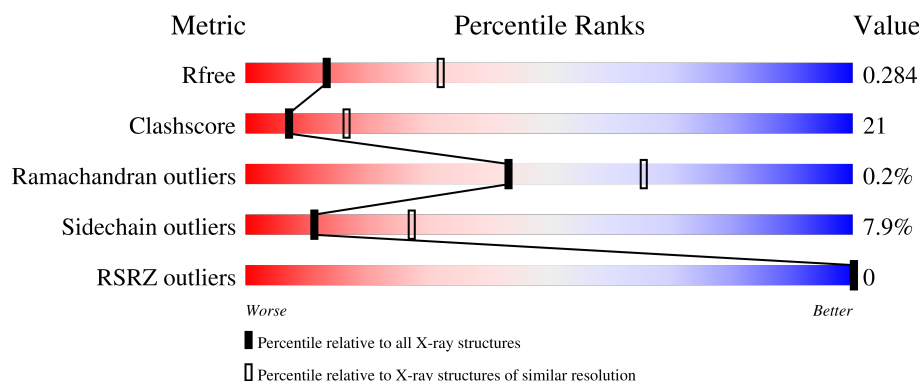
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	560	
1	B	560	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7163 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 Ubiquitin carboxyl-terminal hydrolase 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	1
			3570	2292	600	662	16			
1	B	463	Total	C	N	O	S	0	0	1
			3577	2300	600	662	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	-	expression tag	UNP Q9UHP3
A	156	PRO	-	expression tag	UNP Q9UHP3
B	155	GLY	-	expression tag	UNP Q9UHP3
B	156	PRO	-	expression tag	UNP Q9UHP3

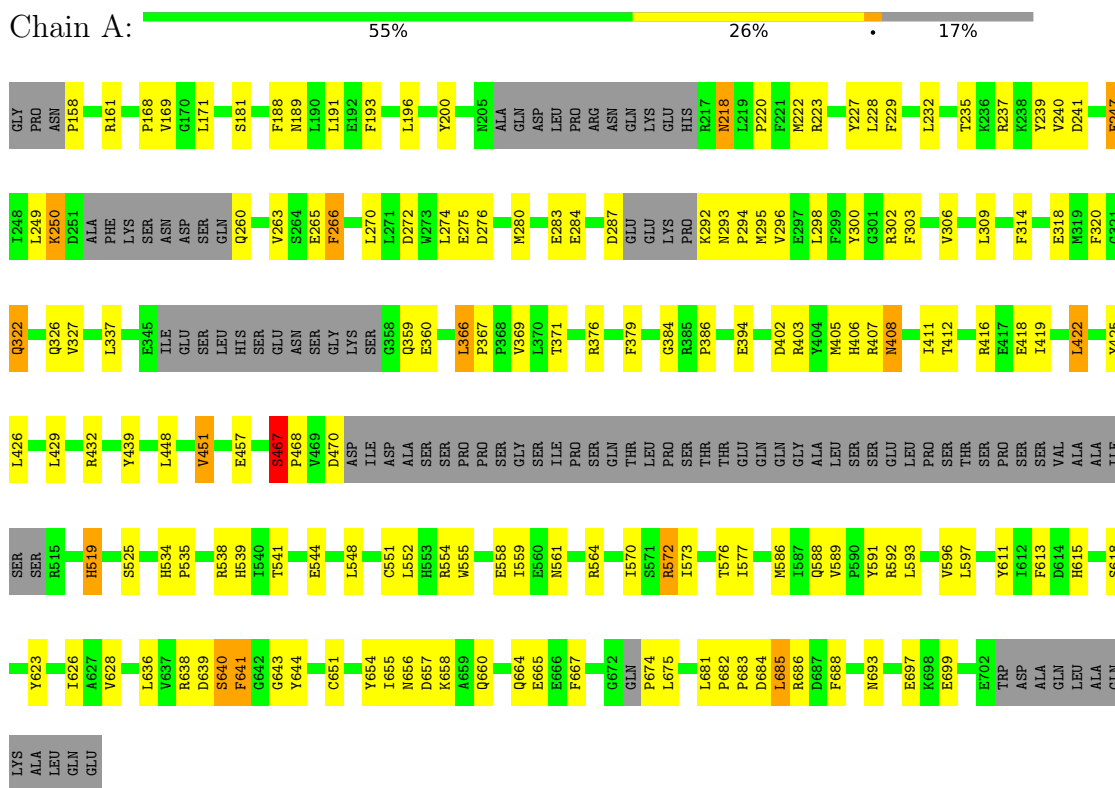
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	9	Total	O	0	0
			9	9		

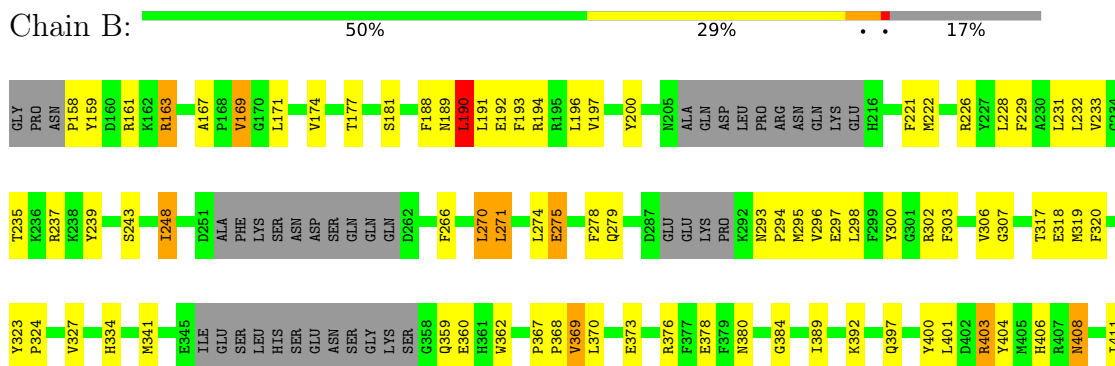
3 Residue-property plots

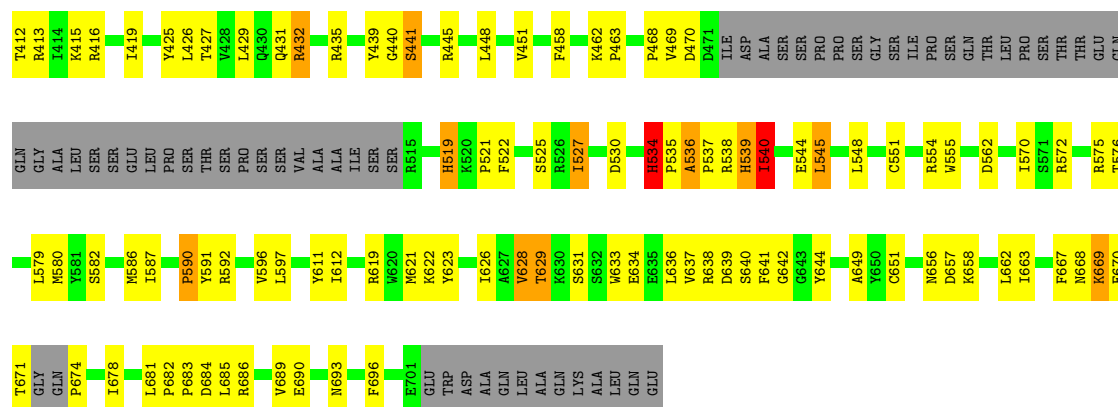
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ubiquitin carboxyl-terminal hydrolase 25



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 25





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	139.18Å 139.18Å 190.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.17 – 2.94 59.17 – 2.94	Depositor EDS
% Data completeness (in resolution range)	54.5 (59.17-2.94) 54.6 (59.17-2.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.13_2998), REFMAC	Depositor
R, R_{free}	0.254 , 0.278 0.258 , 0.284	Depositor DCC
R_{free} test set	1037 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	103.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 138.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.005 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.012 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.013 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.428 for -h,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7163	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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	0.26	0/3659	0.57	6/4983 (0.1%)
1	B	0.28	0/3668	0.64	9/4994 (0.2%)
All	All	0.27	0/7327	0.61	15/9977 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ALA	CA-C-N	11.14	131.11	119.85
1	B	536	ALA	C-N-CA	11.14	131.11	119.85
1	A	467	SER	CA-C-N	10.72	130.95	119.05
1	A	467	SER	C-N-CA	10.72	130.95	119.05
1	A	643	GLY	N-CA-C	-7.73	105.17	115.21
1	A	640	SER	N-CA-C	7.34	119.36	111.36
1	B	527	ILE	N-CA-C	-6.54	102.54	108.95
1	B	190	LEU	N-CA-C	-6.41	100.17	109.59
1	B	534	HIS	N-CA-C	6.23	122.16	113.57
1	B	628	VAL	N-CA-C	-6.14	98.68	107.77
1	B	540	ILE	N-CA-C	5.75	121.31	109.34
1	A	284	GLU	CB-CA-C	-5.59	110.14	116.63
1	A	641	PHE	N-CA-C	5.43	117.19	111.28
1	B	167	ALA	CA-C-N	5.11	125.04	119.78
1	B	167	ALA	C-N-CA	5.11	125.04	119.78

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	3570	0	3206	120	0
1	B	3577	0	3231	178	0
2	A	7	0	0	1	0
2	B	9	0	0	0	0
All	All	7163	0	6437	282	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 21.

All (282) 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:467:SER:CB	1:A:468:PRO:HD3	1.42	1.41
1:B:468:PRO:HA	1:B:534:HIS:NE2	1.33	1.40
1:A:467:SER:CB	1:A:468:PRO:CD	2.01	1.31
1:B:334:HIS:CG	1:B:403:ARG:HH22	1.66	1.13
1:B:468:PRO:CA	1:B:534:HIS:NE2	2.22	1.02
1:B:458:PHE:HE1	1:B:535:PRO:O	1.43	0.98
1:B:334:HIS:CG	1:B:403:ARG:NH2	2.37	0.91
1:A:293:ASN:OD1	1:A:294:PRO:HD2	1.70	0.91
1:B:334:HIS:ND1	1:B:403:ARG:NH2	2.20	0.88
1:A:275:GLU:HB3	1:A:295:MET:HE3	1.53	0.87
1:A:467:SER:CB	1:A:468:PRO:HD2	2.04	0.87
1:B:400:TYR:HE1	1:B:590:PRO:HB3	1.41	0.85
1:B:458:PHE:CE1	1:B:535:PRO:O	2.30	0.84
1:B:545:LEU:HD12	1:B:545:LEU:O	1.87	0.75
1:B:169:VAL:HG11	1:B:232:LEU:HB3	1.68	0.74
1:A:551:CYS:HA	1:A:554:ARG:HH11	1.51	0.74
1:B:400:TYR:CE1	1:B:590:PRO:HB3	2.23	0.73
1:B:667:PHE:HD1	1:B:669:LYS:H	1.37	0.73
1:A:237:ARG:NH2	1:A:699:GLU:OE2	2.23	0.72
1:B:468:PRO:HA	1:B:534:HIS:CE1	2.21	0.72
1:B:196:LEU:HD21	1:B:294:PRO:HB2	1.72	0.71
1:B:536:ALA:HB1	1:B:537:PRO:HD2	1.73	0.71
1:A:218:ASN:N	1:A:218:ASN:OD1	2.24	0.71
1:B:623:TYR:CD2	1:B:628:VAL:HG12	2.25	0.70
1:A:293:ASN:HB3	1:A:296:VAL:HG22	1.71	0.70
1:B:586:MET:HE2	1:B:586:MET:HA	1.72	0.70
1:B:592:ARG:NH1	1:B:657:ASP:OD2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ILE:C	1:B:540:ILE:HD12	2.16	0.70
1:B:682:PRO:HG2	1:B:685:LEU:HD23	1.74	0.70
1:B:392:LYS:HA	1:B:642:GLY:HA3	1.73	0.69
1:A:539:HIS:O	1:B:554:ARG:NH2	2.24	0.69
1:A:403:ARG:O	1:A:412:THR:HG21	1.93	0.68
1:B:200:TYR:H	1:B:226:ARG:HH12	1.42	0.68
1:A:287:ASP:O	1:A:292:LYS:N	2.27	0.67
1:B:689:VAL:O	1:B:693:ASN:ND2	2.28	0.67
1:A:682:PRO:HD2	1:A:685:LEU:HD23	1.77	0.66
1:B:378:GLU:HG3	1:B:389:ILE:HD13	1.77	0.66
1:B:596:VAL:HG21	1:B:636:LEU:HD21	1.78	0.66
1:A:470:ASP:CB	1:B:432:ARG:HH22	2.09	0.65
1:A:158:PRO:HG3	1:A:699:GLU:HG2	1.79	0.65
1:A:558:GLU:OE1	1:B:539:HIS:HE1	1.80	0.65
1:B:408:ASN:ND2	1:B:586:MET:HE1	2.12	0.65
1:B:169:VAL:HG11	1:B:232:LEU:HA	1.78	0.64
1:A:592:ARG:NH1	1:A:657:ASP:OD2	2.31	0.64
1:B:468:PRO:CA	1:B:534:HIS:CE1	2.79	0.63
1:B:169:VAL:HG11	1:B:232:LEU:CB	2.29	0.63
1:A:322:GLN:HA	1:A:371:THR:O	1.99	0.63
1:B:228:LEU:O	1:B:232:LEU:CG	2.47	0.63
1:A:411:ILE:H	1:A:411:ILE:HD12	1.64	0.62
1:B:231:LEU:O	1:B:235:THR:HG22	1.99	0.62
1:A:402:ASP:OD1	1:A:588:GLN:N	2.33	0.62
1:A:161:ARG:NH1	1:A:699:GLU:OE1	2.32	0.61
1:B:197:VAL:HG12	1:B:278:PHE:HZ	1.66	0.61
1:A:309:LEU:HD23	1:A:309:LEU:H	1.66	0.60
1:B:678:ILE:HD12	1:B:678:ILE:H	1.66	0.60
1:A:306:VAL:HG13	1:A:359:GLN:HA	1.84	0.60
1:A:558:GLU:CD	1:B:539:HIS:HE1	2.09	0.60
1:B:519:HIS:NE2	1:B:525:SER:HB3	2.17	0.60
1:A:555:TRP:NE1	1:B:539:HIS:NE2	2.49	0.59
1:B:587:ILE:O	1:B:587:ILE:HG22	2.00	0.59
1:B:200:TYR:O	1:B:226:ARG:NH1	2.35	0.59
1:B:303:PHE:O	1:B:317:THR:HA	2.02	0.59
1:B:392:LYS:NZ	1:B:644:TYR:OH	2.23	0.59
1:B:222:MET:HE1	1:B:274:LEU:HD22	1.85	0.59
1:B:534:HIS:N	1:B:535:PRO:HD2	2.18	0.59
1:B:306:VAL:CG1	1:B:360:GLU:H	2.15	0.59
1:A:684:ASP:OD2	1:A:684:ASP:N	2.35	0.59
1:B:622:LYS:HB3	1:B:629:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HG11	1:B:232:LEU:CA	2.34	0.58
1:A:558:GLU:OE1	1:B:539:HIS:CE1	2.57	0.58
1:B:169:VAL:CG1	1:B:232:LEU:HB3	2.34	0.57
1:B:163:ARG:HB2	1:B:237:ARG:C	2.29	0.57
1:B:174:VAL:H	1:B:177:THR:HG22	1.68	0.57
1:B:619:ARG:NH1	1:B:631:SER:O	2.37	0.57
1:A:250:LYS:O	1:A:250:LYS:HG2	2.04	0.57
1:B:302:ARG:HA	1:B:318:GLU:O	2.04	0.57
1:B:633:TRP:O	1:B:637:VAL:HG13	2.05	0.57
1:A:555:TRP:CD1	1:B:539:HIS:HE2	2.23	0.57
1:B:540:ILE:O	1:B:540:ILE:HG23	2.04	0.57
1:B:271:LEU:O	1:B:275:GLU:HG2	2.04	0.56
1:A:426:LEU:HD11	1:A:570:ILE:HG23	1.87	0.56
1:B:611:TYR:CG	1:B:636:LEU:HD23	2.40	0.56
1:A:247:GLU:OE2	1:A:247:GLU:HA	2.03	0.56
1:B:298:LEU:HA	1:B:368:PRO:HD2	1.88	0.56
1:B:416:ARG:O	1:B:419:ILE:HG12	2.05	0.56
1:B:190:LEU:HD21	1:B:369:VAL:HG11	1.88	0.56
1:B:302:ARG:N	1:B:320:PHE:HE2	2.02	0.56
1:B:368:PRO:O	1:B:591:TYR:HE2	1.88	0.56
1:B:302:ARG:CG	1:B:317:THR:HB	2.36	0.55
1:B:411:ILE:O	1:B:415:LYS:N	2.38	0.55
1:B:668:ASN:ND2	1:B:671:THR:OG1	2.33	0.55
1:B:169:VAL:HG21	1:B:235:THR:CG2	2.36	0.55
1:A:416:ARG:O	1:A:419:ILE:HG12	2.06	0.55
1:A:551:CYS:HA	1:A:554:ARG:NH1	2.21	0.55
1:B:628:VAL:O	1:B:628:VAL:HG23	2.07	0.55
1:B:334:HIS:CD2	1:B:403:ARG:HH22	2.22	0.54
1:A:327:VAL:HG21	1:A:376:ARG:HG2	1.89	0.54
1:B:188:PHE:HB2	1:B:229:PHE:CE1	2.43	0.54
1:A:235:THR:OG1	1:A:237:ARG:HG3	2.07	0.53
1:A:439:TYR:CG	1:A:448:LEU:HD12	2.44	0.53
1:B:306:VAL:HG13	1:B:359:GLN:HA	1.90	0.53
1:A:220:PRO:O	1:A:223:ARG:HG3	2.08	0.53
1:A:656:ASN:OD1	1:A:658:LYS:N	2.38	0.53
1:B:367:PRO:O	1:B:591:TYR:OH	2.26	0.53
1:B:463:PRO:CG	1:B:540:ILE:HG21	2.38	0.53
1:A:320:PHE:CG	1:A:320:PHE:O	2.62	0.53
1:B:158:PRO:HD2	1:B:161:ARG:HB3	1.91	0.53
1:B:637:VAL:O	1:B:641:PHE:HB2	2.09	0.53
1:B:426:LEU:HD21	1:B:570:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:HD22	1:A:559:ILE:HG13	1.92	0.52
1:A:572:ARG:O	1:A:576:THR:HG23	2.09	0.52
1:B:323:TYR:HD1	1:B:324:PRO:HD2	1.74	0.52
1:A:406:HIS:O	1:A:406:HIS:ND1	2.43	0.52
1:B:334:HIS:CE1	1:B:403:ARG:NH2	2.78	0.52
1:A:432:ARG:NH2	1:B:469:VAL:HA	2.25	0.51
1:B:306:VAL:O	1:B:359:GLN:HB2	2.10	0.51
1:B:403:ARG:O	1:B:412:THR:HG21	2.11	0.51
1:B:197:VAL:HG12	1:B:278:PHE:CZ	2.46	0.51
1:A:306:VAL:CG1	1:A:360:GLU:H	2.24	0.51
1:B:684:ASP:OD2	1:B:684:ASP:N	2.41	0.51
1:A:366:LEU:HD13	1:A:591:TYR:OH	2.10	0.50
1:A:555:TRP:CD1	1:B:539:HIS:NE2	2.80	0.50
1:A:660:GLN:O	1:A:664:GLN:HG2	2.11	0.50
1:B:640:SER:OG	1:B:649:ALA:HB2	2.12	0.50
1:A:470:ASP:CB	1:B:432:ARG:NH2	2.74	0.50
1:A:457:GLU:OE2	1:B:441:SER:OG	2.22	0.50
1:B:376:ARG:O	1:B:389:ILE:HG12	2.12	0.50
1:B:226:ARG:HE	1:B:685:LEU:HD21	1.77	0.50
1:B:303:PHE:CE2	1:B:320:PHE:HB3	2.46	0.50
1:B:521:PRO:HB2	1:B:522:PHE:CD2	2.46	0.50
1:B:306:VAL:HG22	1:B:307:GLY:H	1.75	0.50
1:B:226:ARG:NE	1:B:685:LEU:HD21	2.27	0.49
1:A:554:ARG:HG3	1:B:539:HIS:NE2	2.27	0.49
1:B:370:LEU:HD23	1:B:401:LEU:HD11	1.94	0.49
1:B:406:HIS:ND1	1:B:406:HIS:O	2.44	0.49
1:A:296:VAL:HA	1:A:300:TYR:CD1	2.47	0.49
1:A:302:ARG:HA	1:A:318:GLU:O	2.12	0.49
1:A:551:CYS:CA	1:A:554:ARG:HH11	2.22	0.49
1:B:545:LEU:HD12	1:B:545:LEU:C	2.33	0.49
1:B:612:ILE:HG12	1:B:623:TYR:CE1	2.48	0.49
1:A:405:MET:HE2	1:A:405:MET:HB3	1.76	0.49
1:B:296:VAL:HA	1:B:300:TYR:CD1	2.47	0.49
1:B:293:ASN:HB3	1:B:296:VAL:HG22	1.93	0.48
1:B:611:TYR:OH	1:B:639:ASP:OD1	2.30	0.48
1:B:538:ARG:HG3	1:B:539:HIS:ND1	2.28	0.48
1:B:685:LEU:O	1:B:689:VAL:HG23	2.14	0.48
1:A:272:ASP:HA	1:A:275:GLU:OE2	2.12	0.48
1:A:615:HIS:HE1	1:A:655:ILE:HD11	1.79	0.48
1:B:575:ARG:O	1:B:579:LEU:HG	2.13	0.48
1:A:250:LYS:NZ	1:A:250:LYS:CB	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HB2	1:B:662:LEU:HA	1.96	0.48
1:B:298:LEU:O	1:B:369:VAL:HG22	2.13	0.48
1:A:593:LEU:HD13	1:A:654:TYR:CZ	2.49	0.48
1:A:168:PRO:HB2	1:A:628:VAL:HG11	1.96	0.48
1:B:397:GLN:HG2	1:B:633:TRP:CZ3	2.49	0.47
1:B:408:ASN:HD22	1:B:586:MET:HE1	1.79	0.47
1:B:194:ARG:HA	1:B:197:VAL:HG22	1.96	0.47
1:B:306:VAL:HG12	1:B:360:GLU:H	1.80	0.47
1:B:668:ASN:HD22	1:B:674:PRO:N	2.12	0.47
1:B:303:PHE:CE2	1:B:318:GLU:HB2	2.50	0.47
1:A:538:ARG:HH12	1:B:562:ASP:CG	2.22	0.47
1:A:665:GLU:HB3	1:A:675:LEU:CB	2.45	0.47
1:B:341:MET:O	1:B:360:GLU:HA	2.14	0.47
1:B:221:PHE:HB2	1:B:248:ILE:CG2	2.44	0.47
1:A:265:GLU:OE2	1:A:265:GLU:HA	2.15	0.47
1:B:462:LYS:O	1:B:536:ALA:CB	2.63	0.47
1:A:448:LEU:O	1:A:451:VAL:HG22	2.15	0.46
1:B:293:ASN:O	1:B:297:GLU:HG2	2.15	0.46
1:A:558:GLU:OE2	1:B:539:HIS:HE1	1.97	0.46
1:A:228:LEU:O	1:A:232:LEU:HG	2.16	0.46
1:A:296:VAL:HA	1:A:300:TYR:HD1	1.80	0.46
1:B:298:LEU:O	1:B:367:PRO:HB2	2.16	0.46
1:B:572:ARG:O	1:B:576:THR:HG23	2.15	0.46
1:A:239:TYR:CG	1:A:626:ILE:HG13	2.51	0.46
1:B:239:TYR:CG	1:B:626:ILE:HG13	2.50	0.46
1:B:668:ASN:OD1	1:B:670:GLU:N	2.47	0.46
1:B:591:TYR:CZ	1:B:656:ASN:HB2	2.50	0.46
1:B:439:TYR:CG	1:B:448:LEU:HD12	2.51	0.46
1:B:413:ARG:HA	1:B:416:ARG:HB2	1.97	0.45
1:A:379:PHE:HA	1:A:386:PRO:HA	1.98	0.45
1:B:412:THR:O	1:B:416:ARG:N	2.37	0.45
1:A:623:TYR:CD2	1:A:628:VAL:HG22	2.51	0.45
1:B:306:VAL:HG22	1:B:307:GLY:N	2.31	0.45
1:A:266:PHE:HD1	1:A:266:PHE:HA	1.67	0.45
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.77	0.45
1:A:200:TYR:CE2	1:A:222:MET:HG2	2.51	0.45
1:B:634:GLU:HA	1:B:637:VAL:HG22	1.98	0.45
1:A:298:LEU:O	1:A:367:PRO:HB2	2.17	0.45
1:A:561:ASN:HA	1:A:564:ARG:HG2	1.98	0.45
1:B:302:ARG:N	1:B:320:PHE:CE2	2.84	0.45
1:B:637:VAL:HA	1:B:641:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASP:CG	1:A:589:VAL:HG12	2.41	0.45
1:A:596:VAL:HG21	1:A:636:LEU:HD21	1.99	0.45
1:A:169:VAL:HG22	1:A:239:TYR:HA	1.99	0.45
1:A:227:TYR:HD2	1:A:688:PHE:HD1	1.65	0.44
1:B:403:ARG:HD2	1:B:404:TYR:CZ	2.52	0.44
1:B:638:ARG:O	1:B:644:TYR:HB2	2.17	0.44
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.44
1:A:613:PHE:CE1	1:A:618:SER:HA	2.52	0.44
1:B:634:GLU:O	1:B:637:VAL:HG22	2.17	0.44
1:A:306:VAL:HA	1:A:314:PHE:O	2.17	0.44
1:A:379:PHE:HE1	1:A:384:GLY:C	2.26	0.44
1:B:637:VAL:HG12	1:B:641:PHE:CE2	2.51	0.44
1:A:573:ILE:O	1:A:577:ILE:HG13	2.17	0.44
1:A:419:ILE:HA	1:A:422:LEU:HB2	1.99	0.44
1:B:360:GLU:HG3	1:B:362:TRP:HE1	1.82	0.44
1:A:597:LEU:HD13	1:A:651:CYS:HB3	2.00	0.44
1:B:237:ARG:HE	1:B:696:PHE:CB	2.30	0.44
1:A:303:PHE:CE2	1:A:320:PHE:HB3	2.53	0.44
1:B:686:ARG:O	1:B:690:GLU:HG3	2.17	0.44
1:B:427:THR:O	1:B:431:GLN:HG3	2.18	0.43
1:A:223:ARG:O	1:A:227:TYR:HD1	2.00	0.43
1:A:535:PRO:HG3	1:B:435:ARG:HB3	1.99	0.43
1:B:360:GLU:HG3	1:B:362:TRP:NE1	2.34	0.43
1:A:193:PHE:HE1	1:A:295:MET:SD	2.40	0.43
1:B:656:ASN:OD1	1:B:658:LYS:N	2.49	0.43
1:A:275:GLU:HB3	1:A:295:MET:CE	2.37	0.43
1:A:685:LEU:HD21	2:A:803:HOH:O	2.17	0.43
1:A:394:GLU:HA	1:A:641:PHE:CE1	2.54	0.43
1:A:408:ASN:OD1	1:A:408:ASN:N	2.46	0.43
1:A:519:HIS:NE2	1:A:525:SER:HB3	2.34	0.43
1:A:369:VAL:HG22	1:A:655:ILE:HG22	2.01	0.43
1:A:171:LEU:HD12	1:A:181:SER:HA	2.00	0.43
1:A:534:HIS:N	1:A:535:PRO:HD2	2.34	0.43
1:B:231:LEU:O	1:B:235:THR:CG2	2.66	0.43
1:B:323:TYR:OH	1:B:341:MET:HG2	2.19	0.43
1:A:683:PRO:HA	1:A:686:ARG:HB3	2.01	0.42
1:B:376:ARG:HD2	1:B:389:ILE:O	2.19	0.42
1:B:462:LYS:HE3	1:B:530:ASP:O	2.19	0.42
1:A:394:GLU:HG2	1:A:641:PHE:CE1	2.54	0.42
1:A:425:TYR:HE1	1:A:429:LEU:HD11	1.85	0.42
1:B:591:TYR:CE2	1:B:656:ASN:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD23	1:A:665:GLU:HG2	2.00	0.42
1:A:276:ASP:O	1:A:280:MET:HG3	2.19	0.42
1:A:551:CYS:HB2	1:A:555:TRP:CZ3	2.54	0.42
1:B:324:PRO:HA	1:B:373:GLU:HB3	2.00	0.42
1:B:551:CYS:HB3	1:B:555:TRP:CZ3	2.54	0.42
1:A:227:TYR:HD2	1:A:688:PHE:CD1	2.38	0.42
1:B:296:VAL:HA	1:B:300:TYR:HD1	1.85	0.42
1:B:448:LEU:O	1:B:451:VAL:HG22	2.19	0.42
1:B:683:PRO:HA	1:B:686:ARG:HB3	2.01	0.42
1:A:270:LEU:O	1:A:274:LEU:HG	2.19	0.42
1:A:611:TYR:OH	1:A:639:ASP:OD1	2.27	0.42
1:B:425:TYR:HE1	1:B:429:LEU:HD11	1.84	0.42
1:B:171:LEU:HD12	1:B:181:SER:HA	2.02	0.42
1:B:193:PHE:O	1:B:197:VAL:HG13	2.19	0.42
1:B:158:PRO:HB2	1:B:159:TYR:H	1.61	0.42
1:A:394:GLU:HG2	1:A:641:PHE:HE1	1.85	0.41
1:B:468:PRO:HB3	1:B:534:HIS:CE1	2.54	0.41
1:B:306:VAL:HG11	1:B:360:GLU:HG2	2.01	0.41
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.90	0.41
1:B:270:LEU:HG	1:B:271:LEU:HD13	2.02	0.41
1:A:240:VAL:HG22	1:A:241:ASP:H	1.85	0.41
1:A:541:THR:O	1:A:544:GLU:HG2	2.20	0.41
1:A:611:TYR:CG	1:A:636:LEU:HD23	2.55	0.41
1:B:306:VAL:CG2	1:B:307:GLY:H	2.33	0.41
1:A:196:LEU:HD21	1:A:294:PRO:HB2	2.02	0.41
1:B:193:PHE:HE1	1:B:295:MET:SD	2.44	0.41
1:B:221:PHE:HB2	1:B:248:ILE:HG21	2.01	0.41
1:B:222:MET:HE2	1:B:222:MET:HB2	1.91	0.41
1:B:320:PHE:O	1:B:320:PHE:CD1	2.73	0.41
1:B:462:LYS:CE	1:B:530:ASP:O	2.68	0.41
1:B:380:ASN:O	1:B:384:GLY:N	2.52	0.41
1:B:440:GLY:O	1:B:445:ARG:NH1	2.54	0.41
1:B:463:PRO:HG3	1:B:540:ILE:HG21	2.02	0.41
1:B:582:SER:O	1:B:582:SER:OG	2.38	0.41
1:A:586:MET:HE2	1:A:586:MET:HA	2.03	0.41
1:A:589:VAL:HG13	1:A:589:VAL:O	2.20	0.41
1:A:674:PRO:HB2	1:A:675:LEU:H	1.68	0.41
1:B:191:LEU:CD2	1:B:663:ILE:O	2.69	0.41
1:B:597:LEU:HD13	1:B:651:CYS:HB3	2.02	0.41
1:B:163:ARG:HB2	1:B:237:ARG:O	2.20	0.41
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:HB2	1:A:229:PHE:CE1	2.55	0.40
1:A:554:ARG:HG3	1:B:539:HIS:HE2	1.85	0.40
1:A:667:PHE:HA	1:A:674:PRO:HA	2.03	0.40
1:A:693:ASN:O	1:A:697:GLU:HG2	2.21	0.40
1:B:392:LYS:O	1:B:392:LYS:HG3	2.21	0.40
1:B:403:ARG:HD2	1:B:404:TYR:CE2	2.56	0.40
1:B:638:ARG:HA	1:B:644:TYR:HD1	1.87	0.40
1:A:638:ARG:HA	1:A:644:TYR:HD1	1.86	0.40
1:B:200:TYR:CE2	1:B:222:MET:HG2	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	451/560 (80%)	433 (96%)	17 (4%)	1 (0%)	43	65
1	B	449/560 (80%)	428 (95%)	20 (4%)	1 (0%)	43	65
All	All	900/1120 (80%)	861 (96%)	37 (4%)	2 (0%)	43	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	B	590	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	344/507 (68%)	322 (94%)	22 (6%)	16	36
1	B	348/507 (69%)	315 (90%)	33 (10%)	8	21
All	All	692/1014 (68%)	637 (92%)	55 (8%)	11	27

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	218	ASN
1	A	247	GLU
1	A	249	LEU
1	A	250	LYS
1	A	260	GLN
1	A	263	VAL
1	A	266	PHE
1	A	283	GLU
1	A	322	GLN
1	A	326	GLN
1	A	366	LEU
1	A	407	ARG
1	A	408	ASN
1	A	418	GLU
1	A	422	LEU
1	A	451	VAL
1	A	519	HIS
1	A	572	ARG
1	A	640	SER
1	A	681	LEU
1	A	685	LEU
1	B	163	ARG
1	B	169	VAL
1	B	189	ASN
1	B	190	LEU
1	B	233	VAL
1	B	243	SER
1	B	248	ILE
1	B	266	PHE
1	B	270	LEU
1	B	271	LEU
1	B	275	GLU

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Mol	Chain	Res	Type
1	B	279	GLN
1	B	319	MET
1	B	327	VAL
1	B	369	VAL
1	B	403	ARG
1	B	408	ASN
1	B	432	ARG
1	B	441	SER
1	B	470	ASP
1	B	519	HIS
1	B	527	ILE
1	B	534	HIS
1	B	539	HIS
1	B	540	ILE
1	B	544	GLU
1	B	545	LEU
1	B	548	LEU
1	B	580	MET
1	B	621	MET
1	B	629	THR
1	B	669	LYS
1	B	681	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	A	607	HIS
1	A	624	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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	465/560 (83%)	-1.39	0 100 100	39, 77, 114, 144	0
1	B	463/560 (82%)	-1.38	0 100 100	36, 78, 111, 136	0
All	All	928/1120 (82%)	-1.38	0 100 100	36, 78, 112, 144	0

There are no RSRZ outliers to report.

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.