



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 6HEJ / pdb_00006hej
Title : Structure of human USP28
Authors : Gersch, M.; Komander, D.
Deposited on : 2018-08-20
Resolution : 2.79 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

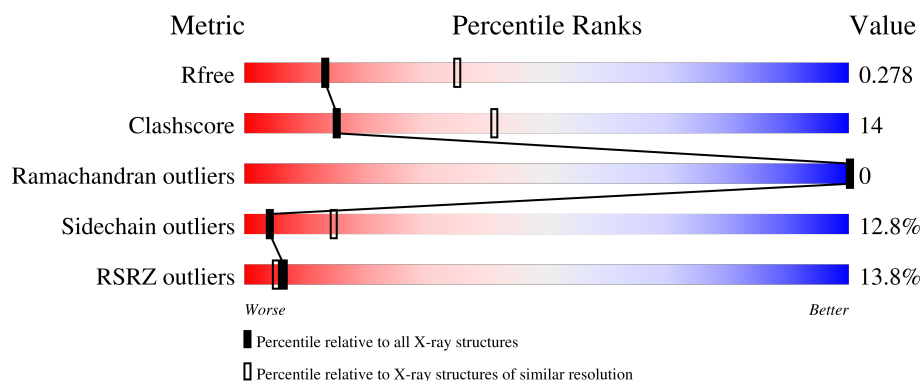
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	556	8% 52% 21% 5% 22%
1	B	556	13% 55% 17% • 26%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6531 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.

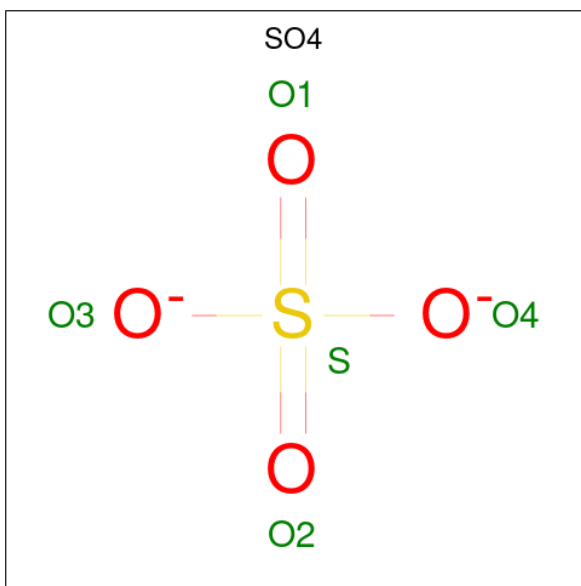
- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3373	2170	558	628	17			
1	B	409	Total	C	N	O	S	0	0	0
			3078	1985	504	571	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	-	expression tag	UNP Q96RU2
B	148	GLY	-	expression tag	UNP Q96RU2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5 4 1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

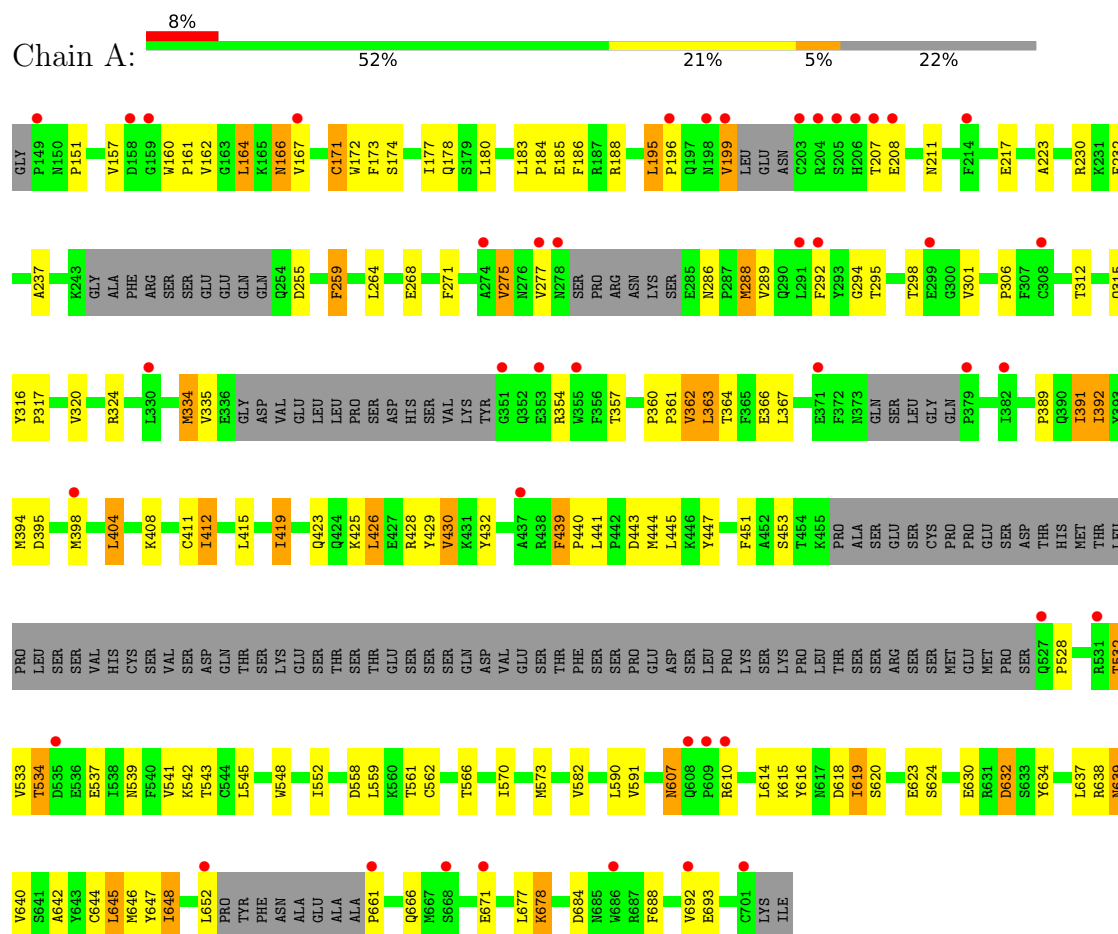
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	32	Total	O	0	0
			32	32		

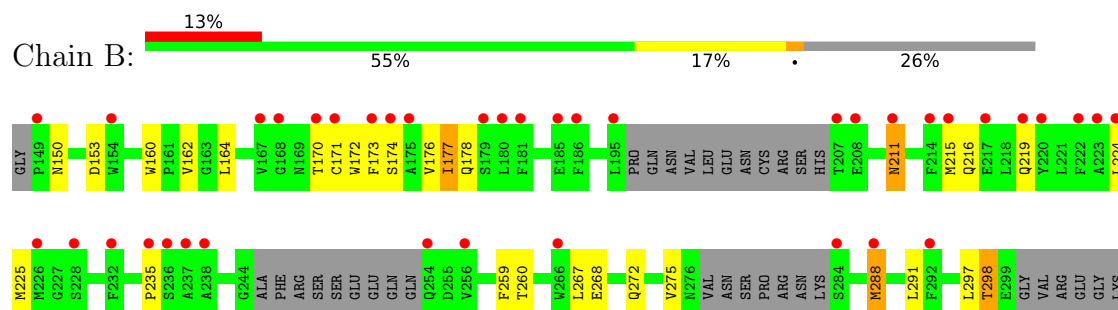
3 Residue-property plots

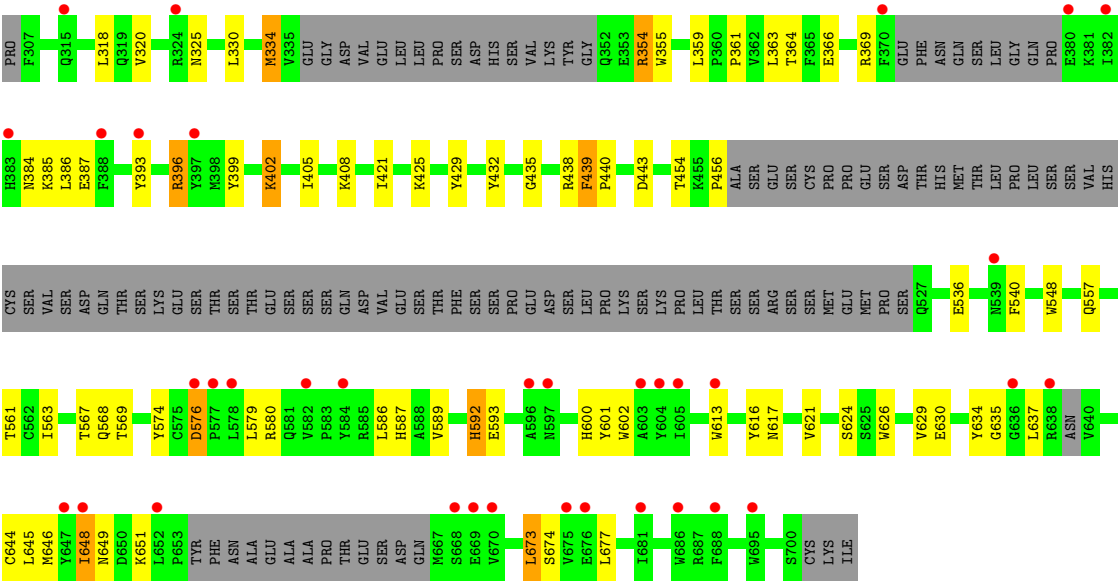
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 28



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 28





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	104.23Å 200.46Å 206.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.84 – 2.79 71.84 – 2.79	Depositor EDS
% Data completeness (in resolution range)	58.8 (71.84-2.79) 58.8 (71.84-2.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.13_2998), RESTRAIN	Depositor
R, R_{free}	0.261 , 0.286 0.262 , 0.278	Depositor DCC
R_{free} test set	1594 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	102.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6531	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.30	0/3456	0.49	0/4708
1	B	0.22	0/3151	0.43	0/4297
All	All	0.26	0/6607	0.46	0/9005

There are no bond length outliers.

There are no bond angle outliers.

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	3373	0	3040	104	0
1	B	3078	0	2704	71	0
2	A	10	0	0	0	0
3	A	38	0	0	1	0
3	B	32	0	0	0	0
All	All	6531	0	5744	166	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 14.

All (166) 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:183:LEU:HD21	1:A:362:VAL:HG21	1.52	0.89
1:B:173:PHE:CZ	1:B:177:ILE:HD11	2.09	0.88
1:A:195:LEU:HD12	1:A:196:PRO:HD3	1.55	0.86
1:B:173:PHE:CZ	1:B:177:ILE:CD1	2.64	0.81
1:A:195:LEU:HD12	1:A:196:PRO:CD	2.10	0.81
1:A:440:PRO:HG2	1:A:443:ASP:HB2	1.67	0.76
1:A:171:CYS:O	1:A:174:SER:N	2.21	0.74
1:A:230:ARG:HH21	1:A:688:PHE:HB2	1.53	0.74
1:A:638:ARG:O	1:A:639:ASN:ND2	2.23	0.72
1:B:334:MET:HG3	1:B:354:ARG:HB3	1.72	0.71
1:A:208:GLU:O	1:A:211:ASN:HB2	1.90	0.71
1:A:294:GLY:HA3	1:A:360:PRO:HD3	1.73	0.71
1:A:614:LEU:HB3	1:A:616:TYR:HE2	1.55	0.69
1:A:562:CYS:O	1:A:566:THR:HG22	1.92	0.69
1:B:387:GLU:HA	1:B:634:TYR:CD2	2.28	0.69
1:B:291:LEU:HA	1:B:361:PRO:HD2	1.75	0.68
1:A:614:LEU:HB3	1:A:616:TYR:CE2	2.30	0.67
1:A:298:THR:HG22	1:A:354:ARG:HG3	1.76	0.66
1:B:454:THR:HG22	1:B:456:PRO:HD2	1.78	0.66
1:A:412:ILE:HD11	1:A:570:ILE:HG23	1.77	0.64
1:A:362:VAL:HG23	1:A:648:ILE:HG22	1.81	0.62
1:B:364:THR:HG22	1:B:646:MET:HG2	1.80	0.62
1:A:232:PHE:CB	1:A:619:ILE:HG22	2.29	0.62
1:A:164:LEU:HD21	1:A:177:ILE:HD11	1.82	0.62
1:B:173:PHE:HZ	1:B:177:ILE:HD11	1.61	0.62
1:B:440:PRO:HG2	1:B:443:ASP:HB2	1.84	0.60
1:A:334:MET:HG3	1:A:354:ARG:HB3	1.84	0.60
1:A:607:ASN:HD21	1:A:610:ARG:HG3	1.69	0.58
1:A:528:PRO:HB3	1:B:429:TYR:HE1	1.69	0.58
1:A:275:VAL:O	1:A:275:VAL:HG13	2.03	0.57
1:A:590:LEU:HD12	1:A:644:CYS:HB3	1.85	0.57
1:A:534:THR:HG23	1:A:537:GLU:HB2	1.85	0.57
1:A:196:PRO:HB2	1:A:199:VAL:HG22	1.87	0.57
1:A:532:THR:O	1:A:532:THR:OG1	2.21	0.57
1:A:415:LEU:O	1:A:419:ILE:HG12	2.05	0.56
1:B:586:LEU:HD23	1:B:613:TRP:CH2	2.41	0.56
1:B:387:GLU:HA	1:B:634:TYR:HD2	1.69	0.55
1:A:363:LEU:HB3	1:A:647:TYR:HB2	1.88	0.55
1:B:369:ARG:HH12	1:B:635:GLY:HA3	1.71	0.55
1:B:387:GLU:HA	1:B:634:TYR:CE2	2.42	0.55
1:B:592:HIS:HB2	1:B:601:TYR:CE2	2.42	0.54
1:A:426:LEU:O	1:A:430:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:CD2	1:A:362:VAL:HG11	2.43	0.54
1:B:600:HIS:NE2	1:B:617:ASN:OD1	2.40	0.53
1:A:277:VAL:HG12	1:A:277:VAL:O	2.08	0.53
1:A:364:THR:HG23	1:A:646:MET:HG2	1.90	0.53
1:B:385:LYS:HA	1:B:634:TYR:O	2.09	0.53
1:B:673:LEU:HD23	1:B:674:SER:H	1.74	0.53
1:A:404:LEU:HD22	1:A:408:LYS:HE2	1.90	0.53
1:A:395:ASP:CG	1:A:582:VAL:HG22	2.33	0.53
1:B:586:LEU:HD23	1:B:613:TRP:HH2	1.74	0.52
1:A:439:PHE:CG	1:A:440:PRO:HD2	2.44	0.52
1:B:563:ILE:O	1:B:567:THR:HG23	2.09	0.52
1:A:361:PRO:O	1:A:648:ILE:HA	2.09	0.52
1:A:230:ARG:NH2	1:A:688:PHE:HB2	2.23	0.52
1:B:164:LEU:HD21	1:B:225:MET:HE3	1.92	0.51
1:B:172:TRP:CZ2	1:B:259:PHE:HD1	2.29	0.51
1:A:301:VAL:HA	1:A:306:PRO:HA	1.92	0.51
1:B:267:LEU:O	1:B:288:MET:HE1	2.12	0.50
1:A:591:VAL:HA	1:A:642:ALA:HA	1.93	0.50
1:A:161:PRO:HG2	1:A:616:TYR:OH	2.12	0.50
1:A:164:LEU:HD23	1:A:174:SER:HA	1.92	0.50
1:A:195:LEU:HD12	1:A:196:PRO:HD2	1.93	0.50
1:B:557:GLN:O	1:B:561:THR:HG23	2.12	0.50
1:B:630:GLU:O	1:B:634:TYR:HD1	1.95	0.50
1:B:369:ARG:NH1	1:B:384:ASN:O	2.45	0.49
1:B:359:LEU:HD22	1:B:363:LEU:HD11	1.93	0.49
1:A:232:PHE:CG	1:A:619:ILE:HG22	2.47	0.49
1:A:439:PHE:HB2	1:B:439:PHE:CE1	2.48	0.49
1:A:637:LEU:HB2	1:A:640:VAL:HG12	1.95	0.49
1:B:320:VAL:HG13	1:B:386:LEU:HD23	1.95	0.49
1:B:626:TRP:HD1	1:B:630:GLU:HG3	1.78	0.49
1:B:171:CYS:SG	1:B:171:CYS:O	2.71	0.48
1:A:151:PRO:HB2	1:A:692:VAL:HG22	1.96	0.48
1:B:173:PHE:CZ	1:B:177:ILE:HD12	2.47	0.48
1:A:217:GLU:OE2	1:A:237:ALA:HB1	2.14	0.48
1:A:528:PRO:HG3	1:B:429:TYR:CE1	2.48	0.48
1:A:362:VAL:HG12	1:A:362:VAL:O	2.14	0.48
1:A:439:PHE:HB2	1:B:439:PHE:CD1	2.48	0.48
1:B:673:LEU:HD23	1:B:674:SER:N	2.29	0.48
1:A:184:PRO:O	1:A:188:ARG:HG3	2.14	0.47
1:B:439:PHE:CG	1:B:440:PRO:HD2	2.50	0.47
1:A:271:PHE:CD2	1:A:288:MET:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLY:CA	1:A:360:PRO:HD3	2.44	0.47
1:A:389:PRO:HB2	1:A:392:ILE:HG22	1.97	0.47
1:A:632:ASP:N	1:A:632:ASP:OD1	2.48	0.47
1:A:678:LYS:HE3	1:A:678:LYS:HB2	1.60	0.46
1:B:164:LEU:HB3	1:B:235:PRO:HG3	1.96	0.46
1:A:271:PHE:HB3	1:A:286:ASN:HD21	1.80	0.46
1:A:295:THR:O	1:A:357:THR:OG1	2.22	0.46
1:B:369:ARG:NH1	1:B:635:GLY:HA3	2.29	0.46
1:A:398:MET:CE	1:A:582:VAL:HG21	2.45	0.46
1:A:666:GLN:OE1	1:A:666:GLN:N	2.47	0.46
1:B:649:ASN:OD1	1:B:651:LYS:N	2.49	0.46
1:B:160:TRP:NE1	1:B:621:VAL:O	2.47	0.46
1:A:429:TYR:HD2	1:A:552:ILE:HG23	1.81	0.46
1:A:394:MET:HB3	1:A:394:MET:HE2	1.73	0.45
1:A:425:LYS:HB3	1:A:559:LEU:HD11	1.97	0.45
1:A:661:PRO:HB3	3:A:932:HOH:O	2.16	0.45
1:A:166:ASN:HB2	1:A:618:ASP:CG	2.41	0.45
1:A:180:LEU:HB3	1:A:186:PHE:CE2	2.52	0.45
1:A:447:TYR:OH	1:B:435:GLY:HA3	2.17	0.45
1:A:392:ILE:O	1:A:392:ILE:HG12	2.13	0.45
1:A:432:TYR:CD2	1:A:441:LEU:HD12	2.52	0.45
1:A:537:GLU:HG3	1:B:540:PHE:CZ	2.52	0.45
1:B:320:VAL:HG22	1:B:386:LEU:HG	1.98	0.45
1:A:445:LEU:HD22	1:A:545:LEU:HD22	1.98	0.45
1:B:405:ILE:HD11	1:B:579:LEU:HD21	1.99	0.45
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.84	0.45
1:A:537:GLU:HG3	1:B:540:PHE:HZ	1.81	0.44
1:B:421:ILE:O	1:B:425:LYS:HG3	2.17	0.44
1:A:183:LEU:CD2	1:A:362:VAL:HG21	2.37	0.44
1:A:391:ILE:O	1:A:391:ILE:HG12	2.17	0.44
1:A:533:VAL:HG21	1:B:548:TRP:HE1	1.82	0.44
1:A:439:PHE:HB3	1:A:444:MET:HE3	1.99	0.44
1:B:593:GLU:HB2	1:B:602:TRP:HZ3	1.83	0.44
1:A:178:GLN:HG2	1:A:616:TYR:HD1	1.82	0.44
1:A:317:PRO:HA	1:A:366:GLU:HB2	2.00	0.44
1:A:288:MET:HE3	1:A:288:MET:HB3	1.83	0.43
1:A:429:TYR:CD2	1:A:552:ILE:HG23	2.53	0.43
1:B:268:GLU:HA	1:B:288:MET:HE1	2.00	0.43
1:A:171:CYS:O	1:A:172:TRP:C	2.61	0.43
1:A:316:TYR:HD1	1:A:317:PRO:HD2	1.83	0.43
1:A:315:GLN:N	1:A:315:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:CG	1:A:616:TYR:HD1	2.31	0.43
1:B:602:TRP:HB2	1:B:616:TYR:O	2.19	0.43
1:A:367:LEU:HD11	1:A:645:LEU:HD11	2.00	0.43
1:B:408:LYS:NZ	1:B:576:ASP:OD1	2.27	0.43
1:B:297:LEU:HD23	1:B:298:THR:N	2.33	0.43
1:B:673:LEU:HD22	1:B:677:LEU:HB3	2.01	0.43
1:B:396:ARG:NH1	1:B:574:TYR:HD1	2.17	0.43
1:A:172:TRP:CH2	1:A:259:PHE:HB3	2.54	0.43
1:B:593:GLU:HB2	1:B:602:TRP:CZ3	2.55	0.42
1:A:230:ARG:NH2	1:A:684:ASP:OD1	2.50	0.42
1:A:615:LYS:C	1:A:616:TYR:HD2	2.27	0.42
1:B:216:GLN:HA	1:B:219:GLN:NE2	2.34	0.42
1:B:396:ARG:H	1:B:396:ARG:HG3	1.55	0.42
1:A:268:GLU:HG3	1:A:289:VAL:HG23	2.01	0.42
1:B:297:LEU:N	1:B:355:TRP:O	2.52	0.42
1:A:295:THR:HG22	1:A:312:THR:HG22	2.01	0.42
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.94	0.42
1:B:384:ASN:OD1	1:B:385:LYS:N	2.53	0.42
1:B:162:VAL:O	1:B:178:GLN:NE2	2.47	0.42
1:B:325:ASN:HA	1:B:387:GLU:H	1.84	0.42
1:A:558:ASP:HA	1:A:561:THR:HG22	2.02	0.41
1:A:453:SER:HB3	1:A:542:LYS:CD	2.51	0.41
1:A:630:GLU:HG2	1:A:634:TYR:CE1	2.56	0.41
1:A:223:ALA:HB2	1:A:677:LEU:HD22	2.01	0.41
1:A:411:CYS:O	1:A:415:LEU:HD23	2.21	0.41
1:A:415:LEU:HB3	1:A:570:ILE:HD11	2.01	0.41
1:A:183:LEU:HD21	1:A:362:VAL:CG2	2.38	0.41
1:A:292:PHE:CE2	1:A:362:VAL:HG11	2.56	0.41
1:A:451:PHE:HB2	1:B:432:TYR:CE2	2.56	0.41
1:A:614:LEU:HD23	1:A:623:GLU:HA	2.03	0.41
1:A:426:LEU:HD13	1:A:430:VAL:HG21	2.03	0.41
1:B:150:ASN:O	1:B:153:ASP:HB3	2.21	0.41
1:B:272:GLN:O	1:B:275:VAL:HG22	2.21	0.41
1:B:393:TYR:CD1	1:B:580:ARG:HA	2.56	0.41
1:B:399:TYR:HE2	1:B:402:LYS:HE3	1.85	0.41
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.92	0.41
1:A:324:ARG:H	1:A:324:ARG:HG3	1.48	0.40
1:A:548:TRP:O	1:A:552:ILE:HG12	2.22	0.40
1:B:211:ASN:OD1	1:B:211:ASN:N	2.54	0.40
1:B:172:TRP:HB2	1:B:601:TYR:HD1	1.87	0.40
1:A:171:CYS:O	1:A:173:PHE:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:HIS:HB2	1:B:648:ILE:HG23	2.03	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	420/556 (76%)	408 (97%)	12 (3%)	0	100	100
1	B	389/556 (70%)	374 (96%)	15 (4%)	0	100	100
All	All	809/1112 (73%)	782 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	329/513 (64%)	280 (85%)	49 (15%)	3	10
1	B	286/513 (56%)	256 (90%)	30 (10%)	6	22
All	All	615/1026 (60%)	536 (87%)	79 (13%)	4	15

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	A	160	TRP
1	A	162	VAL
1	A	164	LEU
1	A	166	ASN
1	A	167	VAL
1	A	171	CYS
1	A	185	GLU
1	A	195	LEU
1	A	199	VAL
1	A	207	THR
1	A	255	ASP
1	A	259	PHE
1	A	264	LEU
1	A	275	VAL
1	A	288	MET
1	A	320	VAL
1	A	334	MET
1	A	335	VAL
1	A	362	VAL
1	A	363	LEU
1	A	391	ILE
1	A	392	ILE
1	A	404	LEU
1	A	412	ILE
1	A	419	ILE
1	A	423	GLN
1	A	426	LEU
1	A	428	ARG
1	A	430	VAL
1	A	439	PHE
1	A	532	THR
1	A	534	THR
1	A	539	ASN
1	A	541	VAL
1	A	543	THR
1	A	573	MET
1	A	607	ASN
1	A	619	ILE
1	A	620	SER
1	A	624	SER
1	A	632	ASP
1	A	639	ASN

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Mol	Chain	Res	Type
1	A	645	LEU
1	A	648	ILE
1	A	652	LEU
1	A	671	GLU
1	A	678	LYS
1	A	693	GLU
1	B	170	THR
1	B	174	SER
1	B	176	VAL
1	B	177	ILE
1	B	211	ASN
1	B	215	MET
1	B	260	THR
1	B	288	MET
1	B	298	THR
1	B	318	LEU
1	B	334	MET
1	B	354	ARG
1	B	366	GLU
1	B	396	ARG
1	B	402	LYS
1	B	438	ARG
1	B	439	PHE
1	B	536	GLU
1	B	568	GLN
1	B	569	THR
1	B	576	ASP
1	B	589	VAL
1	B	592	HIS
1	B	624	SER
1	B	629	VAL
1	B	637	LEU
1	B	644	CYS
1	B	645	LEU
1	B	648	ILE
1	B	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	HIS
1	A	384	ASN

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Mol	Chain	Res	Type
1	A	587	HIS
1	A	607	ASN
1	B	539	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	436/556 (78%)	0.74	43 (9%) 13 9	42, 84, 126, 156	0
1	B	409/556 (73%)	1.07	74 (18%) 3 3	40, 97, 138, 150	0
All	All	845/1112 (75%)	0.90	117 (13%) 6 5	40, 89, 134, 156	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652	LEU	6.5
1	B	220	TYR	5.5
1	B	214	PHE	5.2
1	B	578	LEU	5.0
1	A	203	CYS	4.8
1	B	207	THR	4.5
1	A	277	VAL	4.5
1	B	173	PHE	4.4
1	B	222	PHE	4.4
1	B	613	TRP	4.3
1	B	236	SER	4.2
1	B	232	PHE	4.0
1	A	199	VAL	4.0
1	A	206	HIS	3.9
1	B	670	VAL	3.9
1	B	180	LEU	3.9
1	A	353	GLU	3.5
1	B	582	VAL	3.5
1	A	701	CYS	3.4
1	A	382	ILE	3.4
1	B	686	TRP	3.4
1	B	675	VAL	3.4
1	B	224	LEU	3.3
1	B	647	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	638	ARG	3.3
1	B	195	LEU	3.3
1	B	576	ASP	3.2
1	B	223	ALA	3.2
1	B	149	PRO	3.2
1	B	604	TYR	3.2
1	B	254	GLN	3.1
1	B	370	PHE	3.1
1	B	219	GLN	3.1
1	B	669	GLU	3.1
1	B	577	PRO	3.0
1	B	237	ALA	3.0
1	B	266	TRP	3.0
1	B	215	MET	2.9
1	A	205	SER	2.9
1	A	278	ASN	2.9
1	A	159	GLY	2.8
1	B	175	ALA	2.8
1	A	208	GLU	2.8
1	A	292	PHE	2.8
1	A	671	GLU	2.8
1	B	292	PHE	2.8
1	A	198	ASN	2.8
1	A	299	GLU	2.8
1	B	208	GLU	2.8
1	B	324	ARG	2.8
1	B	174	SER	2.7
1	B	168	GLY	2.7
1	B	539	ASN	2.7
1	B	383	HIS	2.7
1	A	274	ALA	2.7
1	B	256	VAL	2.7
1	A	535	ASP	2.7
1	A	371	GLU	2.7
1	B	217	GLU	2.7
1	B	605	ILE	2.6
1	A	351	GLY	2.6
1	B	185	GLU	2.6
1	B	179	SER	2.6
1	A	661	PRO	2.6
1	B	235	PRO	2.6
1	A	167	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	315	GLN	2.6
1	B	584	TYR	2.5
1	A	308	CYS	2.5
1	A	398	MET	2.5
1	A	291	LEU	2.5
1	B	393	TYR	2.5
1	B	186	PHE	2.5
1	B	681	ILE	2.5
1	A	196	PRO	2.5
1	A	692	VAL	2.5
1	B	284	SER	2.4
1	A	527	GLN	2.4
1	A	207	THR	2.4
1	B	211	ASN	2.4
1	B	676	GLU	2.4
1	A	214	PHE	2.4
1	B	380	GLU	2.4
1	B	288	MET	2.4
1	B	228	SER	2.3
1	B	171	CYS	2.3
1	B	668	SER	2.3
1	B	596	ALA	2.3
1	B	226	MET	2.3
1	B	695	TRP	2.3
1	B	167	VAL	2.3
1	B	688	PHE	2.3
1	A	204	ARG	2.2
1	A	608	GLN	2.2
1	B	170	THR	2.2
1	A	668	SER	2.2
1	A	330	LEU	2.2
1	A	531	ARG	2.2
1	B	597	ASN	2.2
1	B	636	GLY	2.2
1	A	158	ASP	2.2
1	B	648	ILE	2.2
1	A	379	PRO	2.1
1	A	609	PRO	2.1
1	B	181	PHE	2.1
1	A	437	ALA	2.1
1	A	355	TRP	2.1
1	A	610	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	686	TRP	2.1
1	B	652	LEU	2.1
1	B	388	PHE	2.1
1	B	238	ALA	2.1
1	B	154	TRP	2.1
1	A	149	PRO	2.1
1	B	382	ILE	2.1
1	B	603	ALA	2.0
1	B	397	TYR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	802	5/5	0.75	0.08	110,117,137,144	0
2	SO4	A	801	5/5	0.89	0.06	97,97,109,110	5

6.5 Other polymers [i](#)

There are no such residues in this entry.