Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:58 am BST

PDB ID	:	6H4H
Title	:	Usp28 catalytic domain variant E593D in complex with UbPA
Authors	:	Klemm, T.A.; Sauer, F.; Kisker, C.
Deposited on	:	2018-07-21
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

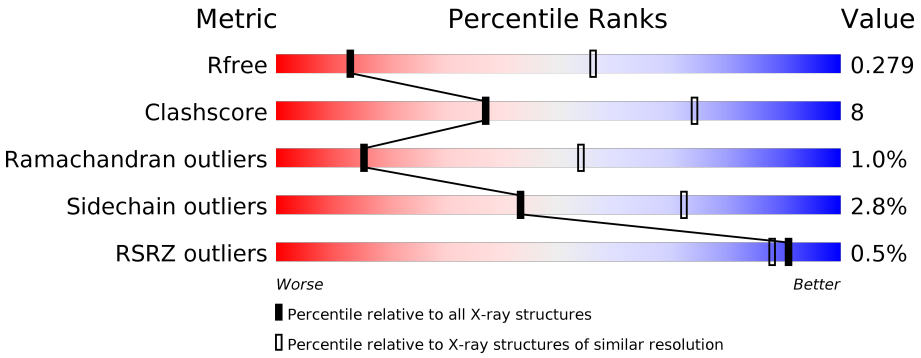
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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 <=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	65% 16% • 18%
1	B	560	% 58% 16% • 25%
2	C	75	84% 16%
2	D	75	% 68% 29% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8378 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	458	Total	C	N	O	S	0	0	0
			3764	2397	638	707	22			
1	B	420	Total	C	N	O	S	0	0	0
			3417	2184	579	635	19			

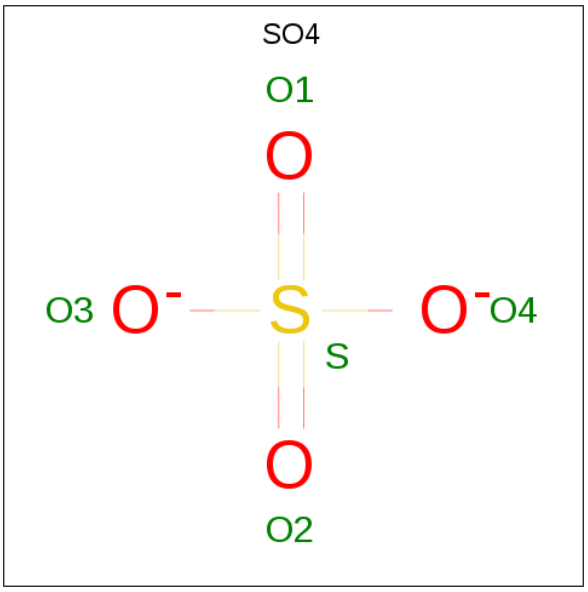
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	-	expression tag	UNP Q96RU2
A	593	ASP	GLU	engineered mutation	UNP Q96RU2
B	148	GLY	-	expression tag	UNP Q96RU2
B	593	ASP	GLU	engineered mutation	UNP Q96RU2

- Molecule 2 is a protein called Polyubiquitin-B.

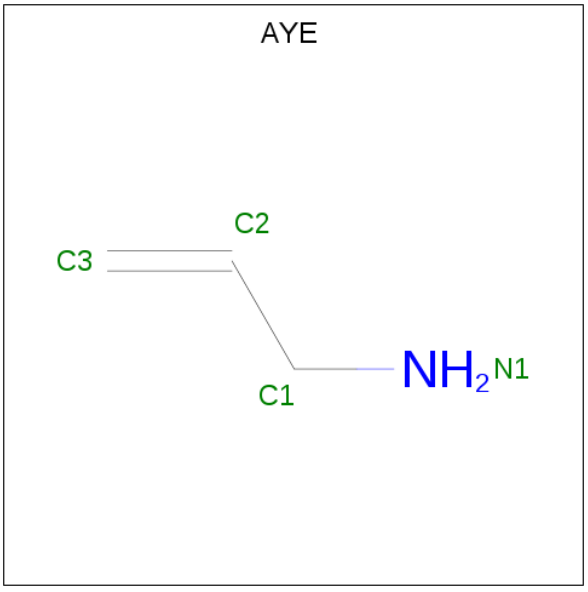
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	D	75	Total	C	N	O	S	0	0	0
			587	370	100	116	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is prop-2-en-1-amine (three-letter code: AYE) (formula: C_3H_7N).



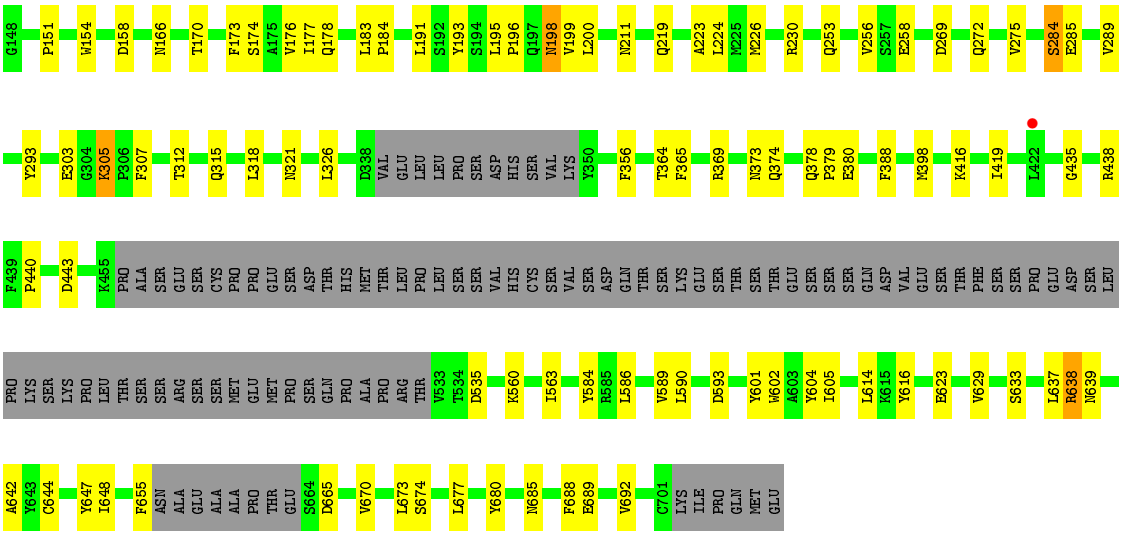
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 4 3 1	0	0
4	B	1	Total C N 4 3 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

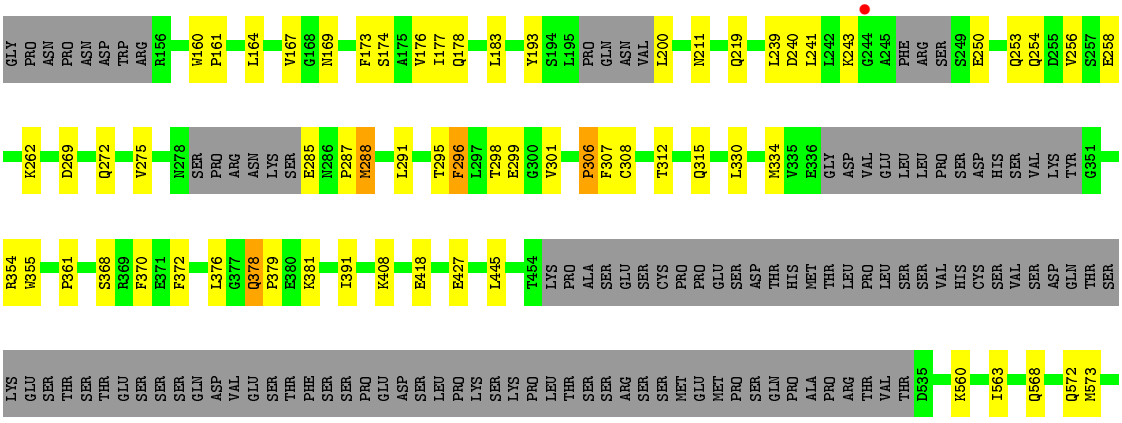
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 28

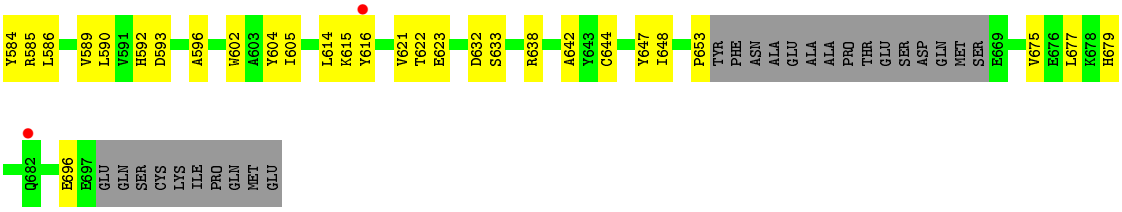
Chain A:



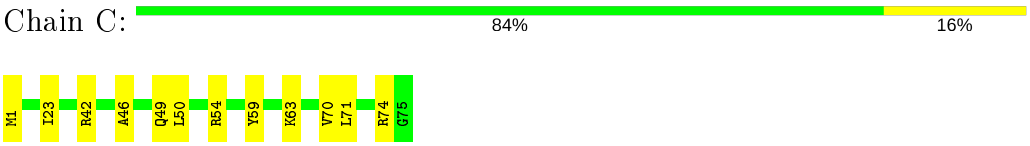
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 28

Chain B:

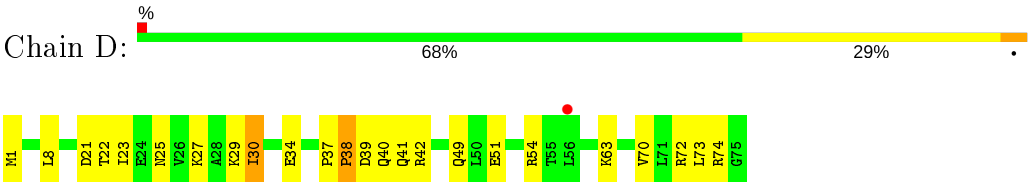




- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	171.75Å 213.64Å 98.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 3.50 49.28 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.28-3.50) 97.6 (49.28-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.232 , 0.280 0.232 , 0.279	Depositor DCC
R_{free} test set	1116 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	98.5	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 106.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8378	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AYE, 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	0.26	0/3855	0.43	0/5216
1	B	0.26	0/3492	0.48	1/4721 (0.0%)
2	C	0.25	0/603	0.52	0/811
2	D	0.26	0/593	0.69	0/800
All	All	0.26	0/8543	0.48	1/11548 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	241	LEU	CA-CB-CG	5.75	128.53	115.30

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	3764	0	3599	56	0
1	B	3417	0	3273	56	0
2	C	597	0	626	9	0
2	D	587	0	604	23	0
3	A	5	0	0	0	0
4	A	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	4	0	0
All	All	8378	0	8111	128	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 8.

All (128) 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:378:GLN:HB3	1:B:379:PRO:HD3	1.55	0.89
1:B:239:LEU:HD23	1:B:239:LEU:O	1.79	0.80
1:B:295:THR:HG22	1:B:312:THR:HG22	1.65	0.79
1:B:378:GLN:HB3	1:B:379:PRO:CD	2.15	0.77
2:C:1:MET:HB2	2:C:63:LYS:HG2	1.68	0.76
2:D:1:MET:HB2	2:D:63:LYS:HG2	1.68	0.75
1:A:258:GLU:HG3	2:C:49:GLN:HE22	1.54	0.72
2:D:38:PRO:O	2:D:40:GLN:N	2.23	0.72
2:D:21:ASP:HB3	2:D:25:ASN:HD21	1.58	0.68
1:B:381:LYS:HD2	2:D:73:LEU:HD11	1.77	0.66
1:A:629:VAL:O	1:A:633:SER:OG	2.13	0.66
1:B:372:PHE:HB2	1:B:376:LEU:HD11	1.79	0.65
1:A:289:VAL:HA	1:A:293:TYR:HD2	1.63	0.63
1:B:378:GLN:HE21	2:D:37:PRO:HG2	1.63	0.63
1:A:191:LEU:HD13	1:A:673:LEU:HD11	1.81	0.62
1:A:258:GLU:HG3	2:C:49:GLN:NE2	2.15	0.62
1:B:596:ALA:HA	2:D:73:LEU:HD13	1.81	0.62
1:A:435:GLY:O	1:A:438:ARG:NH2	2.32	0.62
1:A:284:SER:HB2	1:A:285:GLU:OE1	1.99	0.61
1:A:637:LEU:HG	1:A:638:ARG:HE	1.65	0.61
1:B:169:ASN:HB3	1:B:253:GLN:HE22	1.65	0.61
2:D:38:PRO:C	2:D:40:GLN:H	2.07	0.58
1:B:299:GLU:HA	1:B:308:CYS:HB3	1.86	0.58
1:A:195:LEU:HD12	1:A:196:PRO:HD2	1.84	0.57
1:A:158:ASP:OD2	1:B:408:LYS:NZ	2.37	0.57
1:B:211:ASN:HD22	1:B:269:ASP:HB3	1.68	0.57
1:B:258:GLU:HG3	2:D:49:GLN:HE22	1.69	0.56
1:A:211:ASN:HD22	1:A:269:ASP:HB3	1.71	0.55
1:B:262:LYS:HE2	2:D:51:GLU:HG3	1.89	0.55
1:A:256:VAL:HG11	1:A:590:LEU:HD22	1.89	0.54
1:B:633:SER:HB3	1:B:642:ALA:HB2	1.89	0.54
2:D:27:LYS:O	2:D:41:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:MET:HG2	1:A:670:VAL:HG22	1.90	0.53
1:B:590:LEU:HB2	1:B:644:CYS:HB2	1.89	0.53
1:A:369:ARG:NH1	1:A:642:ALA:O	2.42	0.52
1:B:174:SER:O	1:B:178:GLN:HB2	2.10	0.52
1:A:560:LYS:O	1:A:563:ILE:HG13	2.10	0.52
1:A:315:GLN:HA	1:A:364:THR:HG23	1.91	0.52
1:A:590:LEU:HB2	1:A:644:CYS:HB2	1.91	0.51
1:B:391:ILE:HD12	1:B:391:ILE:O	2.10	0.51
1:A:176:VAL:CG2	1:A:256:VAL:HG13	2.41	0.51
2:D:51:GLU:OE1	2:D:54:ARG:NH2	2.44	0.50
1:B:256:VAL:HG11	1:B:590:LEU:HD22	1.94	0.50
1:B:592:HIS:CE1	2:D:73:LEU:HD12	2.46	0.49
1:B:378:GLN:NE2	2:D:37:PRO:HG2	2.26	0.49
1:A:605:ILE:HD12	1:A:616:TYR:CD1	2.47	0.49
1:A:685:ASN:O	1:A:689:GLU:HG2	2.13	0.49
2:D:29:LYS:O	2:D:30:ILE:HG23	2.11	0.49
1:A:223:ALA:HB2	1:A:677:LEU:HD22	1.95	0.49
1:B:296:PHE:HE2	1:B:354:ARG:HD3	1.78	0.49
1:B:287:PRO:O	1:B:288:MET:HG3	2.12	0.48
1:A:230:ARG:HG3	1:A:688:PHE:CD1	2.49	0.48
1:B:560:LYS:O	1:B:563:ILE:HG13	2.14	0.48
1:A:584:TYR:HB3	1:A:647:TYR:HB3	1.94	0.48
1:A:589:VAL:CG1	1:A:604:TYR:HB2	2.43	0.47
1:B:193:TYR:O	1:B:219:GLN:NE2	2.41	0.47
1:B:275:VAL:HG21	1:B:285:GLU:HA	1.96	0.47
1:A:586:LEU:HD13	1:A:647:TYR:CZ	2.49	0.47
1:B:614:LEU:HD23	1:B:623:GLU:HA	1.97	0.47
1:B:176:VAL:CG2	1:B:256:VAL:HG13	2.45	0.47
1:B:568:GLN:HG2	1:B:572:GLN:NE2	2.30	0.47
1:B:584:TYR:HB3	1:B:647:TYR:HB3	1.97	0.47
2:D:42:ARG:NE	2:D:49:GLN:OE1	2.36	0.47
1:A:253:GLN:O	2:C:74:ARG:HD3	2.15	0.47
1:B:298:THR:HG22	1:B:354:ARG:HG2	1.97	0.47
1:B:160:TRP:N	1:B:161:PRO:HD2	2.30	0.46
2:D:38:PRO:HA	2:D:41:GLN:HG2	1.97	0.46
1:A:183:LEU:HD21	1:A:648:ILE:HD12	1.98	0.46
1:A:230:ARG:HG3	1:A:688:PHE:CE1	2.51	0.46
1:B:378:GLN:NE2	2:D:40:GLN:HB2	2.31	0.46
1:A:174:SER:O	1:A:178:GLN:HB2	2.16	0.46
1:A:224:LEU:HG	1:A:680:TYR:HE2	1.80	0.46
1:A:356:PHE:HB2	1:A:398:MET:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ARG:HH12	1:B:653:PRO:HB2	1.81	0.46
1:B:330:LEU:O	1:B:334:MET:HG2	2.16	0.46
1:A:272:GLN:HA	1:A:275:VAL:HG22	1.98	0.45
1:A:289:VAL:HA	1:A:293:TYR:CD2	2.47	0.45
1:A:318:LEU:HD12	1:A:365:PHE:HB3	1.99	0.45
1:B:178:GLN:HG2	1:B:616:TYR:CD2	2.52	0.45
1:B:593:ASP:HB2	1:B:602:TRP:HZ3	1.81	0.45
1:A:199:VAL:HG23	1:A:200:LEU:HD22	1.99	0.45
1:A:379:PRO:HB3	2:C:71:LEU:HD13	1.98	0.45
2:D:22:THR:N	2:D:25:ASN:OD1	2.49	0.45
1:B:589:VAL:CG1	1:B:604:TYR:HB2	2.47	0.45
1:B:381:LYS:HB3	1:B:596:ALA:HB2	1.99	0.45
1:A:416:LYS:O	1:A:419:ILE:HB	2.18	0.44
1:A:151:PRO:HG2	1:A:692:VAL:HG12	1.99	0.44
1:A:305:LYS:O	1:A:305:LYS:HD2	2.18	0.44
1:B:173:PHE:CZ	1:B:177:ILE:HG13	2.52	0.44
1:B:675:VAL:O	1:B:679:HIS:HB2	2.18	0.43
1:B:254:GLN:O	2:D:74:ARG:HA	2.19	0.43
1:A:198:ASN:ND2	1:A:198:ASN:O	2.51	0.43
1:A:173:PHE:CZ	1:A:177:ILE:HG13	2.54	0.43
1:A:614:LEU:HD23	1:A:623:GLU:HA	2.01	0.43
1:A:166:ASN:OD1	1:A:170:THR:N	2.50	0.43
2:D:27:LYS:HG2	2:D:41:GLN:CD	2.39	0.43
1:A:195:LEU:HG	1:A:199:VAL:HG11	2.01	0.42
1:A:219:GLN:HG2	1:A:677:LEU:HD21	2.00	0.42
1:A:589:VAL:HG13	1:A:604:TYR:HB2	2.01	0.42
1:B:272:GLN:NE2	1:B:287:PRO:HG3	2.34	0.42
1:A:183:LEU:HD23	1:A:184:PRO:HD2	2.01	0.42
1:B:605:ILE:HD12	1:B:616:TYR:CD1	2.54	0.42
1:B:296:PHE:HB2	1:B:355:TRP:O	2.19	0.42
1:A:312:THR:O	2:C:46:ALA:HA	2.19	0.42
2:C:50:LEU:HD22	2:C:59:TYR:CD2	2.55	0.42
1:B:167:VAL:HG21	1:B:239:LEU:HD13	2.01	0.42
1:B:301:VAL:HA	1:B:306:PRO:HA	2.01	0.42
1:A:593:ASP:HB2	1:A:602:TRP:HZ3	1.84	0.42
1:B:368:SER:HA	1:B:370:PHE:CE2	2.55	0.42
2:C:42:ARG:HB2	2:C:70:VAL:HG23	2.01	0.42
1:A:193:TYR:HB3	1:A:219:GLN:NE2	2.34	0.42
1:A:378:GLN:HB3	1:A:379:PRO:HD2	2.01	0.42
1:B:586:LEU:HD13	1:B:647:TYR:CZ	2.55	0.42
2:D:23:ILE:HG12	2:D:54:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:ND2	1:A:380:GLU:OE1	2.52	0.41
1:B:183:LEU:HD21	1:B:648:ILE:HG21	2.02	0.41
1:B:291:LEU:HA	1:B:361:PRO:HD2	2.02	0.41
1:A:388:PHE:HZ	1:A:633:SER:HB2	1.85	0.41
1:A:638:ARG:HB3	1:A:639:ASN:H	1.56	0.41
1:B:164:LEU:HD13	1:B:178:GLN:OE1	2.20	0.41
1:B:243:LYS:HE2	1:B:250:GLU:OE2	2.20	0.41
2:D:42:ARG:HB2	2:D:70:VAL:HG23	2.01	0.41
1:B:615:LYS:HB3	1:B:622:THR:HG22	2.01	0.41
1:B:615:LYS:O	1:B:621:VAL:HA	2.20	0.41
1:B:370:PHE:CE1	2:D:8:LEU:HD22	2.56	0.41
1:A:440:PRO:HG2	1:A:443:ASP:HB2	2.02	0.41
2:C:23:ILE:HG12	2:C:54:ARG:O	2.21	0.41
1:A:256:VAL:HG23	1:A:601:TYR:CE2	2.55	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	450/560 (80%)	425 (94%)	22 (5%)	3 (1%)	22 61
1	B	406/560 (72%)	374 (92%)	29 (7%)	3 (1%)	22 61
2	C	73/75 (97%)	72 (99%)	1 (1%)	0	100 100
2	D	73/75 (97%)	67 (92%)	2 (3%)	4 (6%)	2 17
All	All	1002/1270 (79%)	938 (94%)	54 (5%)	10 (1%)	15 54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	SER

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Mol	Chain	Res	Type
1	B	306	PRO
1	B	378	GLN
2	D	30	ILE
2	D	39	ASP
1	A	321	ASN
1	B	315	GLN
1	A	303	GLU
2	D	38	PRO
2	D	34	GLU

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	409/517 (79%)	398 (97%)	11 (3%)	44 73
1	B	365/517 (71%)	352 (96%)	13 (4%)	35 66
2	C	68/68 (100%)	68 (100%)	0	100 100
2	D	66/68 (97%)	65 (98%)	1 (2%)	65 84
All	All	908/1170 (78%)	883 (97%)	25 (3%)	43 72

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	TRP
1	A	198	ASN
1	A	305	LYS
1	A	307	PHE
1	A	326	LEU
1	A	374	GLN
1	A	535	ASP
1	A	638	ARG
1	A	655	PHE
1	A	665	ASP
1	A	674	SER
1	B	200	LEU

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Mol	Chain	Res	Type
1	B	240	ASP
1	B	288	MET
1	B	296	PHE
1	B	307	PHE
1	B	418	GLU
1	B	427	GLU
1	B	445	LEU
1	B	573	MET
1	B	632	ASP
1	B	638	ARG
1	B	677	LEU
1	B	696	GLU
2	D	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	ASN
1	B	253	GLN
1	B	378	GLN
1	B	572	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
4	AYE	A	802	1,2	3,3,3	0.78	0	1,2,2	1.03	0
3	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
4	AYE	B	801	1,2	3,3,3	0.72	0	1,2,2	1.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AYE	A	802	1,2	-	1/1/1/1	-
4	AYE	B	801	1,2	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	AYE	N1-C1-C2-C3
4	B	801	AYE	N1-C1-C2-C3

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, 95^{th} 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	458/560 (81%)	-0.39	1 (0%)	95	93	64, 121, 211, 250	1 (0%)
1	B	420/560 (75%)	-0.26	3 (0%)	87	83	110, 173, 238, 330	0
2	C	75/75 (100%)	-0.26	0	100	100	85, 149, 196, 214	0
2	D	75/75 (100%)	0.06	1 (1%)	77	71	153, 215, 270, 301	0
All	All	1028/1270 (80%)	-0.30	5 (0%)	91	88	64, 151, 235, 330	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	682	GLN	2.6
1	A	422	LEU	2.2
1	B	244	GLY	2.1
2	D	56	LEU	2.0
1	B	616	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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
3	SO4	A	801	5/5	0.74	0.27	203,209,216,218	0
4	AYE	B	801	4/4	0.91	0.16	110,116,129,141	0
4	AYE	A	802	4/4	0.98	0.20	79,106,106,116	0

6.5 Other polymers (i)

There are no such residues in this entry.