



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:35 PM UTC

PDB ID : 3H69 / pdb_00003h69
Title : Catalytic domain of human Serine/Threonine Phosphatase 5 (PP5c) with two Zn²⁺ atoms complexed with endothall
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Talluri, E.
Deposited on : 2009-04-23
Resolution : 2.10 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

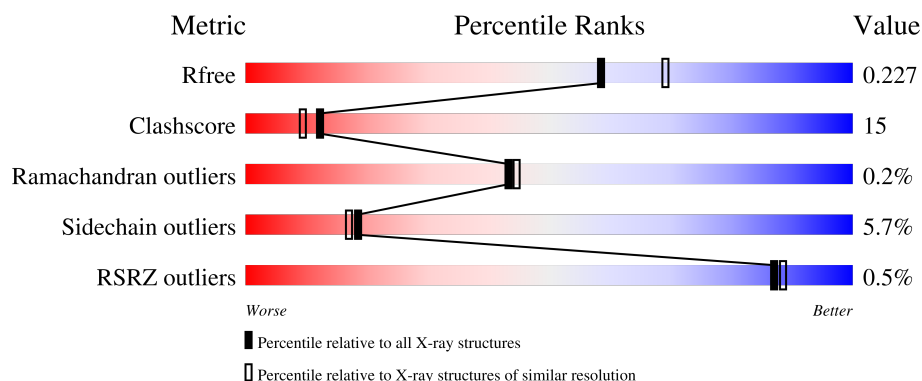
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	315	74% 20% 6%
1	D	315	70% 27% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5433 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.

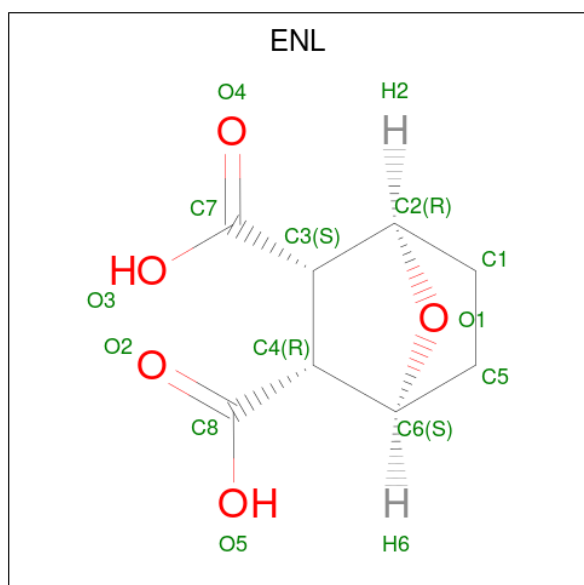
- Molecule 1 is a protein called Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			
1	D	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (1R,2S,3R,4S)-7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid (CCD ID: ENL) (formula: C₈H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			16	9	7		
3	D	1	Total	C	O	0	1
			16	9	7		

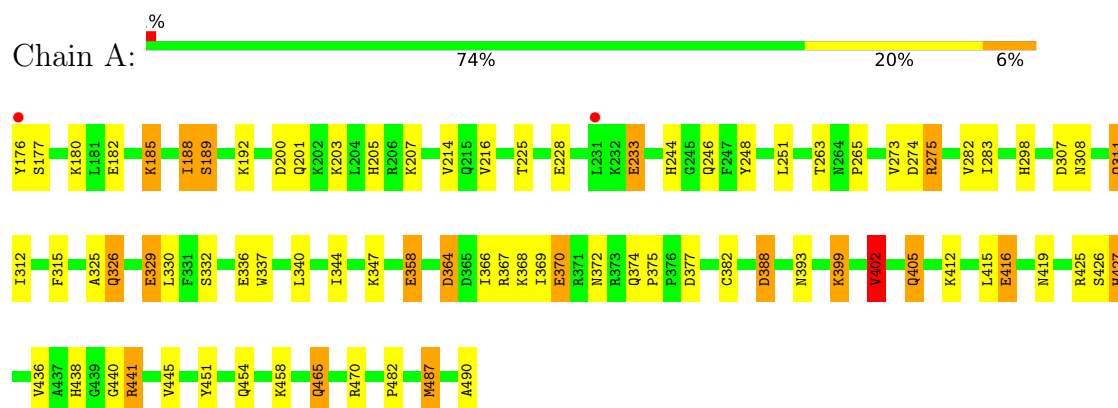
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	D	127	Total	O	0	0
			127	127		

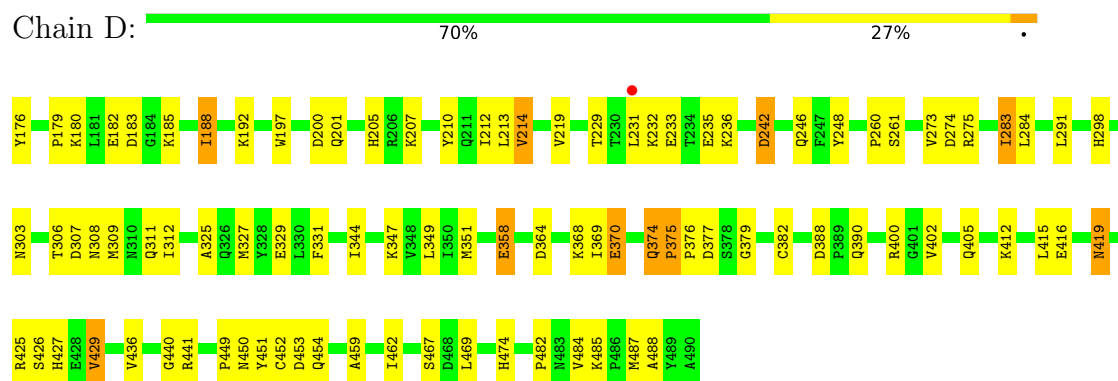
3 Residue-property plots

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: Serine/threonine-protein phosphatase 5



- Molecule 1: Serine/threonine-protein phosphatase 5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.53Å 41.78Å 105.48Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	38.32 – 2.10 38.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.32-2.10) 99.9 (38.32-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.162 , 0.227 0.162 , 0.227	Depositor DCC
R_{free} test set	3585 reflections (9.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% 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: ENL, ZN

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	1.61	21/2592 (0.8%)	1.46	21/3506 (0.6%)
1	D	1.35	8/2592 (0.3%)	1.30	14/3506 (0.4%)
All	All	1.48	29/5184 (0.6%)	1.38	35/7012 (0.5%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	GLU	CG-CD	8.40	1.73	1.52
1	A	337	TRP	N-CA	7.97	1.56	1.46
1	D	429	VAL	CA-CB	7.95	1.63	1.54
1	D	358	GLU	CG-CD	6.89	1.69	1.52
1	D	390	GLN	CA-C	6.87	1.59	1.52
1	A	283	ILE	C-O	6.64	1.32	1.24
1	A	405	GLN	C-O	-6.58	1.16	1.24
1	A	244	HIS	C-O	6.39	1.31	1.23
1	A	189	SER	N-CA	6.25	1.54	1.46
1	A	375	PRO	CA-C	6.22	1.55	1.51
1	D	283	ILE	CA-CB	6.21	1.62	1.54
1	A	330	LEU	CA-C	5.96	1.60	1.52
1	A	251	LEU	C-O	-5.89	1.17	1.24
1	D	382	CYS	CA-C	5.82	1.60	1.52
1	D	306	THR	CA-C	5.75	1.59	1.52
1	A	311	GLN	CG-CD	5.69	1.66	1.52
1	A	416	GLU	N-CA	5.66	1.53	1.46
1	A	388	ASP	N-CA	5.62	1.53	1.45
1	D	462	ILE	CA-CB	5.56	1.61	1.54
1	A	393	ASN	CA-C	5.37	1.60	1.52
1	A	282	VAL	CA-C	-5.35	1.46	1.52
1	A	344	ILE	N-CA	5.32	1.52	1.46
1	A	283	ILE	CA-CB	5.28	1.61	1.54
1	A	445	VAL	C-O	5.17	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ILE	N-CA	5.16	1.52	1.46
1	A	377	ASP	N-CA	-5.13	1.39	1.46
1	D	484	VAL	CA-CB	5.12	1.60	1.54
1	A	402	VAL	C-O	-5.10	1.17	1.23
1	A	458	LYS	N-CA	-5.07	1.39	1.45

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	379	GLY	CA-C-N	13.34	132.84	118.97
1	D	379	GLY	C-N-CA	13.34	132.84	118.97
1	A	470	ARG	CA-C-N	-9.06	110.54	120.14
1	A	470	ARG	C-N-CA	-9.06	110.54	120.14
1	A	233	GLU	N-CA-C	8.47	121.45	111.71
1	A	312	ILE	CB-CA-C	-8.34	101.96	111.55
1	A	375	PRO	N-CA-C	6.97	117.16	110.47
1	A	375	PRO	CA-C-N	-6.91	113.59	120.98
1	A	375	PRO	C-N-CA	-6.91	113.59	120.98
1	A	364	ASP	N-CA-C	6.59	118.46	111.28
1	A	427	HIS	N-CA-CB	-6.51	106.74	114.17
1	D	374	GLN	CA-C-N	-6.43	114.96	119.66
1	D	374	GLN	C-N-CA	-6.43	114.96	119.66
1	D	375	PRO	CA-C-N	-6.41	114.12	120.98
1	D	375	PRO	C-N-CA	-6.41	114.12	120.98
1	D	327	MET	N-CA-C	-6.10	104.71	111.36
1	D	219	VAL	N-CA-C	5.80	115.99	110.42
1	D	312	ILE	CB-CA-C	-5.77	104.67	111.94
1	A	308	ASN	CB-CA-C	-5.70	101.38	110.84
1	D	419	ASN	N-CA-C	5.60	119.16	111.54
1	A	189	SER	CB-CA-C	-5.53	100.05	110.67
1	A	374	GLN	CA-C-N	-5.43	115.69	119.66
1	A	374	GLN	C-N-CA	-5.43	115.69	119.66
1	A	315	PHE	N-CA-C	5.37	116.81	111.07
1	A	244	HIS	N-CA-C	5.27	118.67	111.39
1	D	369	ILE	CA-C-N	-5.24	115.81	122.77
1	D	369	ILE	C-N-CA	-5.24	115.81	122.77
1	D	467	SER	N-CA-C	-5.19	107.00	113.38
1	A	375	PRO	CB-CA-C	-5.14	106.56	111.39
1	A	366	ILE	N-CA-C	-5.13	105.70	110.53
1	A	233	GLU	CB-CG-CD	-5.07	103.97	112.60
1	D	459	ALA	N-CA-C	-5.07	102.05	109.81
1	A	326	GLN	N-CA-C	5.07	116.50	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	TRP	CA-C-N	5.01	127.47	120.65
1	A	337	TRP	C-N-CA	5.01	127.47	120.65

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	2528	0	2462	75	0
1	D	2528	0	2462	81	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	16	0	2	0	0
3	D	16	0	2	0	0
4	A	214	0	0	15	1
4	D	127	0	0	12	1
All	All	5433	0	4928	155	2

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 15.

All (155) 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:D:441:ARG:HG3	4:D:562:HOH:O	1.52	1.08
1:A:275:ARG:HH11	1:A:275:ARG:HG3	1.19	1.03
1:A:275:ARG:HH11	1:A:275:ARG:CG	1.72	1.01
1:A:307:ASP:O	1:A:311:GLN:HG2	1.61	1.00
1:A:412:LYS:HB2	4:A:164:HOH:O	1.65	0.95
1:A:185:LYS:HE2	4:A:126:HOH:O	1.66	0.93
1:A:370:GLU:O	1:A:370:GLU:HG3	1.68	0.93
1:A:176:TYR:HE2	1:A:180:LYS:HE2	1.32	0.92
1:A:176:TYR:CE2	1:A:180:LYS:HE2	2.07	0.90
1:A:185:LYS:CB	4:A:555:HOH:O	2.21	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:O	1:D:311:GLN:HG2	1.72	0.89
1:A:182:GLU:O	1:A:185:LYS:HD2	1.74	0.86
1:A:185:LYS:HB2	4:A:555:HOH:O	1.76	0.85
1:A:182:GLU:O	1:A:185:LYS:CD	2.26	0.84
1:D:307:ASP:HB3	1:D:311:GLN:HE21	1.43	0.83
1:D:205:HIS:HD2	1:D:207:LYS:H	1.28	0.81
1:D:370:GLU:O	1:D:370:GLU:HG3	1.82	0.80
1:D:176:TYR:CE2	1:D:180:LYS:HE3	2.17	0.79
1:D:212:ILE:HG23	1:D:291:LEU:HD12	1.66	0.76
1:D:275:ARG:HH11	1:D:275:ARG:HG3	1.51	0.76
1:A:412:LYS:HG3	1:A:441:ARG:HH21	1.49	0.75
1:A:205:HIS:HD2	1:A:207:LYS:H	1.32	0.75
1:A:412:LYS:NZ	1:A:416:GLU:OE2	2.19	0.73
1:D:176:TYR:HE2	1:D:180:LYS:CE	2.01	0.73
1:A:412:LYS:HD2	4:A:164:HOH:O	1.88	0.71
1:D:416:GLU:CG	4:D:543:HOH:O	2.39	0.70
1:A:228:GLU:OE2	1:A:367:ARG:NH1	2.25	0.70
1:D:248:TYR:CE1	1:D:482:PRO:HD2	2.26	0.70
1:A:487:MET:HG3	1:A:490:ALA:HB2	1.74	0.68
1:D:412:LYS:NZ	1:D:416:GLU:OE2	2.27	0.68
1:A:382:CYS:SG	1:A:402:VAL:CG2	2.83	0.67
1:A:233:GLU:OE2	4:A:557:HOH:O	2.12	0.67
1:A:233:GLU:O	4:A:571:HOH:O	2.14	0.66
1:D:273:VAL:O	1:D:274:ASP:HB2	1.96	0.65
1:D:376:PRO:HG2	4:D:565:HOH:O	1.95	0.65
1:D:416:GLU:HG3	4:D:543:HOH:O	1.95	0.65
1:A:370:GLU:O	1:A:370:GLU:CG	2.42	0.65
1:A:176:TYR:HB3	4:A:584:HOH:O	1.96	0.65
1:A:275:ARG:NH1	1:A:275:ARG:HG3	2.03	0.64
1:D:205:HIS:CD2	1:D:207:LYS:H	2.14	0.64
1:A:273:VAL:O	1:A:274:ASP:HB2	1.97	0.64
1:D:182:GLU:O	1:D:183:ASP:HB2	1.98	0.64
1:A:176:TYR:CE2	1:A:180:LYS:CE	2.80	0.63
1:A:205:HIS:CD2	1:A:207:LYS:H	2.12	0.63
1:A:182:GLU:O	1:A:185:LYS:HD3	1.98	0.63
1:D:307:ASP:HB3	1:D:311:GLN:NE2	2.13	0.63
1:A:275:ARG:NH1	1:A:275:ARG:CG	2.46	0.63
1:D:349:LEU:HD23	1:D:351:MET:HE1	1.80	0.62
1:A:185:LYS:HB3	4:A:555:HOH:O	1.89	0.62
1:D:176:TYR:HE2	1:D:180:LYS:HE3	1.59	0.62
1:D:388:ASP:O	1:D:405:GLN:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:ARG:CG	4:D:562:HOH:O	2.26	0.61
1:A:200:ASP:O	1:A:201:GLN:HB2	2.00	0.60
1:D:364:ASP:OD2	1:D:368:LYS:NZ	2.31	0.59
1:D:176:TYR:CE2	1:D:180:LYS:CE	2.82	0.59
1:D:325:ALA:O	1:D:329:GLU:HG2	2.02	0.59
1:A:364:ASP:OD2	1:A:368:LYS:NZ	2.32	0.58
1:D:176:TYR:CD2	1:D:180:LYS:HE3	2.39	0.58
1:D:416:GLU:HG2	4:D:543:HOH:O	2.01	0.58
1:A:246:GLN:HE22	1:A:451:TYR:HA	1.70	0.57
1:A:382:CYS:SG	1:A:402:VAL:HG23	2.44	0.57
1:D:200:ASP:O	1:D:201:GLN:HB2	2.05	0.56
1:A:326:GLN:HB2	4:A:175:HOH:O	2.05	0.56
1:A:347:LYS:HE2	4:A:544:HOH:O	2.05	0.56
1:A:274:ASP:O	1:A:275:ARG:HB2	2.05	0.55
1:D:212:ILE:HG23	1:D:291:LEU:CD1	2.34	0.55
1:A:188:ILE:C	1:A:188:ILE:HD13	2.32	0.55
1:D:436:VAL:CG1	1:D:440:GLY:HA2	2.37	0.54
1:A:176:TYR:CD2	1:A:180:LYS:CE	2.91	0.54
1:D:441:ARG:NE	4:D:562:HOH:O	1.90	0.54
1:D:229:THR:HB	1:D:344:ILE:HD13	1.90	0.54
1:A:388:ASP:O	1:A:405:GLN:HA	2.10	0.52
1:A:307:ASP:HB3	1:A:311:GLN:NE2	2.24	0.52
1:A:325:ALA:O	1:A:329:GLU:HG2	2.10	0.52
1:D:205:HIS:CD2	1:D:207:LYS:HG3	2.45	0.52
1:D:233:GLU:HG2	4:D:558:HOH:O	2.10	0.51
1:D:298:HIS:HE1	4:D:158:HOH:O	1.94	0.51
1:D:441:ARG:NH2	4:D:543:HOH:O	2.44	0.50
1:A:298:HIS:HD2	4:A:25:HOH:O	1.94	0.50
1:D:349:LEU:HD23	1:D:351:MET:CE	2.41	0.50
1:A:188:ILE:HD11	1:A:192:LYS:HE3	1.93	0.50
1:A:188:ILE:HD11	1:A:192:LYS:CE	2.43	0.49
1:D:260:PRO:O	1:D:261:SER:HB3	2.12	0.49
1:A:438:HIS:O	1:A:441:ARG:HG2	2.12	0.48
1:D:248:TYR:CE1	1:D:482:PRO:CD	2.96	0.48
1:D:275:ARG:HH11	1:D:275:ARG:CG	2.16	0.47
1:A:336:GLU:O	1:A:372:ASN:HA	2.13	0.47
1:D:415:LEU:CD1	1:D:441:ARG:HD2	2.45	0.47
1:D:303:ASN:O	1:D:309:MET:HG3	2.15	0.47
1:A:225:THR:HG21	1:A:369:ILE:HB	1.97	0.46
1:A:399:LYS:HE2	4:A:585:HOH:O	2.16	0.46
1:A:436:VAL:CG1	1:A:440:GLY:HA2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:HE2	1:A:487:MET:HB2	1.72	0.46
1:D:284:LEU:HD23	1:D:284:LEU:HA	1.85	0.46
1:A:225:THR:CG2	1:A:340:LEU:HD12	2.46	0.46
1:D:452:CYS:O	1:D:453:ASP:HB2	2.16	0.46
1:A:307:ASP:HB3	1:A:311:GLN:HE21	1.81	0.45
1:A:228:GLU:CD	1:A:367:ARG:NH1	2.74	0.45
1:D:487:MET:HB2	1:D:487:MET:HE2	1.68	0.45
1:A:307:ASP:OD1	1:A:332:SER:OG	2.28	0.44
1:D:358:GLU:CG	4:D:10:HOH:O	2.65	0.44
1:D:415:LEU:HD11	1:D:441:ARG:HB3	2.00	0.44
1:D:210:TYR:CZ	1:D:214:VAL:HG11	2.52	0.44
1:A:454:GLN:NE2	1:D:454:GLN:NE2	2.65	0.44
1:A:412:LYS:CB	4:A:164:HOH:O	2.42	0.44
1:A:465:GLN:HB2	4:A:571:HOH:O	2.17	0.44
1:A:426:SER:O	1:A:427:HIS:HB3	2.17	0.43
1:D:232:LYS:HD2	1:D:235:GLU:CD	2.43	0.43
1:D:201:GLN:NE2	1:D:482:PRO:HB3	2.33	0.43
1:A:248:TYR:CZ	1:A:482:PRO:HD3	2.54	0.43
1:D:487:MET:O	1:D:488:ALA:C	2.60	0.42
1:D:176:TYR:HE2	1:D:180:LYS:HE2	1.79	0.42
1:D:188:ILE:HD11	1:D:192:LYS:HE3	2.01	0.42
1:A:263:THR:C	1:A:265:PRO:HD3	2.44	0.42
1:A:415:LEU:HD11	1:A:441:ARG:HB3	2.01	0.42
1:D:182:GLU:O	1:D:183:ASP:CB	2.67	0.41
1:D:469:LEU:HD23	1:D:469:LEU:HA	1.88	0.41
1:D:347:LYS:HD3	1:D:347:LYS:HA	1.66	0.41
1:D:188:ILE:HD13	1:D:188:ILE:O	2.21	0.41
1:D:213:LEU:HD21	1:D:331:PHE:CE1	2.56	0.41
1:D:246:GLN:HE22	1:D:451:TYR:HA	1.85	0.41
1:D:248:TYR:CZ	1:D:482:PRO:CD	3.03	0.41
1:D:179:PRO:HD3	1:D:197:TRP:CG	2.56	0.41
1:D:179:PRO:HD3	1:D:197:TRP:CD2	2.56	0.41
1:D:242:ASP:OD1	1:D:426:SER:HB3	2.21	0.41
1:D:351:MET:HE3	1:D:351:MET:HB3	1.96	0.41
1:D:275:ARG:NH1	1:D:275:ARG:CG	2.80	0.41
1:D:374:GLN:O	1:D:375:PRO:C	2.62	0.41
1:A:329:GLU:HG2	1:A:329:GLU:H	1.78	0.40
1:D:449:PRO:O	1:D:450:ASN:C	2.64	0.40
1:D:474:HIS:HB3	4:D:82:HOH:O	2.20	0.40
1:A:188:ILE:HD13	1:A:188:ILE:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:86:HOH:O	4:A:518:HOH:O[4_544]	2.13	0.07
4:D:83:HOH:O	4:D:563:HOH:O[4_545]	2.14	0.06

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	313/315 (99%)	298 (95%)	15 (5%)	0	100	100
1	D	313/315 (99%)	295 (94%)	17 (5%)	1 (0%)	36	36
All	All	626/630 (99%)	593 (95%)	32 (5%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	308	ASN

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	279/279 (100%)	261 (94%)	18 (6%)	15	13
1	D	279/279 (100%)	265 (95%)	14 (5%)	22	22
All	All	558/558 (100%)	526 (94%)	32 (6%)	18	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	SER
1	A	185	LYS
1	A	188	ILE
1	A	189	SER
1	A	203	LYS
1	A	214	VAL
1	A	216	VAL
1	A	275	ARG
1	A	329	GLU
1	A	358	GLU
1	A	370	GLU
1	A	399	LYS
1	A	402	VAL
1	A	419	ASN
1	A	425	ARG
1	A	441	ARG
1	A	465	GLN
1	A	487	MET
1	D	185	LYS
1	D	188	ILE
1	D	214	VAL
1	D	231	LEU
1	D	236	LYS
1	D	242	ASP
1	D	283	ILE
1	D	370	GLU
1	D	377	ASP
1	D	402	VAL
1	D	419	ASN
1	D	425	ARG
1	D	429	VAL
1	D	485	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	246	GLN
1	A	264	ASN
1	A	298	HIS
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	405	GLN
1	A	454	GLN
1	A	465	GLN
1	A	474	HIS
1	D	201	GLN
1	D	205	HIS
1	D	211	GLN
1	D	246	GLN
1	D	264	ASN
1	D	296	HIS
1	D	298	HIS
1	D	310	ASN
1	D	311	GLN
1	D	390	GLN
1	D	405	GLN
1	D	454	GLN
1	D	465	GLN
1	D	474	HIS

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	ENL	D	0[A]	2	14,14,14	1.66	3 (21%)	21,21,21	2.72	6 (28%)
3	ENL	D	0[B]	2	14,14,14	1.61	3 (21%)	21,21,21	3.43	7 (33%)
3	ENL	A	0[A]	2	14,14,14	1.66	3 (21%)	21,21,21	3.86	13 (61%)
3	ENL	A	0[B]	2	14,14,14	1.47	2 (14%)	21,21,21	4.13	15 (71%)

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
3	ENL	D	0[A]	2	-	1/8/29/29	0/3/2/2
3	ENL	D	0[B]	2	-	0/8/29/29	0/3/2/2
3	ENL	A	0[A]	2	-	0/8/29/29	0/3/2/2
3	ENL	A	0[B]	2	-	0/8/29/29	0/3/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	0[A]	ENL	O2-C8	4.08	1.34	1.22
3	A	0[A]	ENL	O2-C8	3.87	1.33	1.22
3	D	0[B]	ENL	O2-C8	3.63	1.32	1.22
3	A	0[B]	ENL	O2-C8	3.38	1.32	1.22
3	D	0[A]	ENL	C3-C7	-3.18	1.44	1.51
3	D	0[B]	ENL	C3-C7	-3.18	1.44	1.51
3	A	0[A]	ENL	O1-C6	-3.02	1.38	1.45
3	A	0[B]	ENL	O1-C6	-3.02	1.38	1.45
3	A	0[A]	ENL	O5-C8	-2.89	1.21	1.30
3	D	0[B]	ENL	O5-C8	-2.59	1.22	1.30
3	D	0[A]	ENL	O5-C8	-2.58	1.22	1.30

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	0[A]	ENL	C2-C3-C7	-9.37	84.15	111.96
3	A	0[B]	ENL	C2-C3-C7	-9.37	84.15	111.96
3	D	0[B]	ENL	C6-C4-C8	-8.03	88.14	111.96
3	D	0[A]	ENL	C2-C3-C7	-8.00	88.22	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	O[B]	ENL	C2-C3-C7	-8.00	88.22	111.96
3	A	O[A]	ENL	C1-C2-C3	7.52	117.75	109.69
3	A	O[B]	ENL	C1-C2-C3	7.52	117.75	109.69
3	A	O[B]	ENL	C3-C4-C8	-7.16	98.56	115.07
3	D	O[B]	ENL	C3-C4-C8	5.96	128.82	115.07
3	A	O[A]	ENL	O4-C7-C3	5.46	136.80	122.84
3	A	O[B]	ENL	O4-C7-C3	5.46	136.80	122.84
3	D	O[A]	ENL	C5-C6-C4	-5.19	104.13	109.69
3	D	O[B]	ENL	C5-C6-C4	-5.19	104.13	109.69
3	A	O[A]	ENL	C4-C3-C7	5.19	127.03	115.07
3	A	O[B]	ENL	C4-C3-C7	5.19	127.03	115.07
3	A	O[A]	ENL	O3-C7-O4	-4.75	113.31	124.08
3	A	O[B]	ENL	O3-C7-O4	-4.75	113.31	124.08
3	D	O[A]	ENL	C4-C3-C7	4.60	125.68	115.07
3	D	O[B]	ENL	C4-C3-C7	4.60	125.68	115.07
3	A	O[A]	ENL	C4-C3-C2	-3.96	95.85	101.40
3	A	O[B]	ENL	C4-C3-C2	-3.96	95.85	101.40
3	A	O[A]	ENL	C6-C4-C8	-3.66	101.09	111.96
3	D	O[A]	ENL	C5-C1-C2	-3.27	96.79	103.14
3	D	O[B]	ENL	C5-C1-C2	-3.27	96.79	103.14
3	A	O[A]	ENL	C5-C6-C4	3.24	113.16	109.69
3	A	O[B]	ENL	C5-C6-C4	3.24	113.16	109.69
3	A	O[A]	ENL	C5-C1-C2	-3.10	97.13	103.14
3	A	O[B]	ENL	C5-C1-C2	-3.10	97.13	103.14
3	A	O[B]	ENL	O5-C8-C4	2.81	121.99	113.91
3	A	O[A]	ENL	O1-C6-C5	-2.80	99.61	104.34
3	A	O[B]	ENL	O1-C6-C5	-2.80	99.61	104.34
3	A	O[A]	ENL	C3-C4-C6	2.79	105.32	101.40
3	A	O[B]	ENL	C3-C4-C6	2.79	105.32	101.40
3	A	O[A]	ENL	C3-C4-C8	2.61	121.08	115.07
3	D	O[A]	ENL	C3-C4-C6	-2.31	98.17	101.40
3	D	O[B]	ENL	C3-C4-C6	-2.31	98.17	101.40
3	A	O[A]	ENL	O1-C6-C4	-2.29	98.74	103.34
3	A	O[B]	ENL	O1-C6-C4	-2.29	98.74	103.34
3	A	O[B]	ENL	O5-C8-O2	-2.15	119.20	124.08
3	A	O[B]	ENL	C6-C4-C8	2.12	118.23	111.96
3	D	O[A]	ENL	O5-C8-C4	2.12	120.00	113.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	0[A]	ENL	C6-C4-C8-O2

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 [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	315/315 (100%)	-0.58	2 (0%) 85 87	9, 18, 33, 50	4 (1%)
1	D	315/315 (100%)	-0.27	1 (0%) 90 91	14, 27, 47, 61	4 (1%)
All	All	630/630 (100%)	-0.43	3 (0%) 87 88	9, 23, 42, 61	8 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	2.9
1	A	231	LEU	2.1
1	A	176	TYR	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](#)

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
3	ENL	D	0[A]	13/13	0.91	0.14	28,38,47,48	3
3	ENL	D	0[B]	13/13	0.91	0.14	35,39,47,48	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ENL	A	0[A]	13/13	0.93	0.12	22,28,35,40	3
3	ENL	A	0[B]	13/13	0.93	0.12	22,30,35,40	3
2	ZN	A	501	1/1	0.99	0.01	5,5,5,5	0
2	ZN	D	500	1/1	1.00	0.02	7,7,7,7	0
2	ZN	D	501	1/1	1.00	0.01	7,7,7,7	0
2	ZN	A	500	1/1	1.00	0.01	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.