



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 PM UTC

PDB ID : 9B0B / pdb_00009b0b
Title : Structure of Optineurin bound to HOIP NZF1 domain
Authors : Michel, M.A.; Scutts, S.; Komander, D.
Deposited on : 2024-03-11
Resolution : 1.70 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:

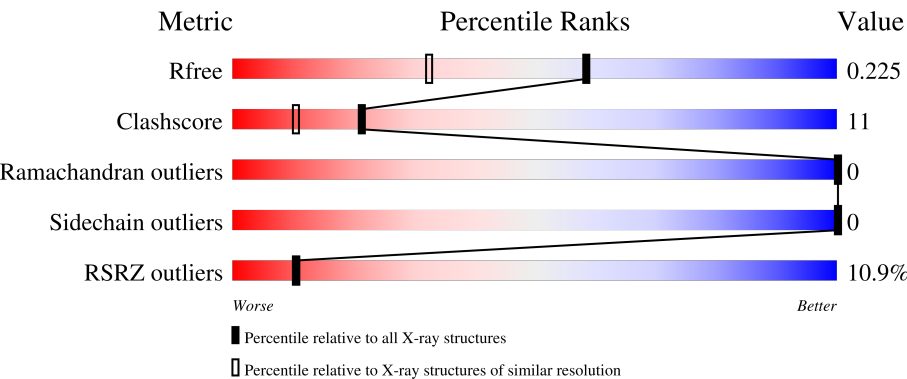
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	96	6% 76%11%11%
1	B	96	11% 67%18%14%
1	C	96	14% 68%19%14%
1	D	96	9% 78%11%10%
2	E	30	3% 87%10%

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Mol	Chain	Length	Quality of chain
2	G	30	10% 90% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3638 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 Optineurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	6	0
			701	440	115	140	6			
1	B	83	Total	C	N	O	S	0	6	0
			696	434	117	140	5			
1	C	83	Total	C	N	O	S	0	4	0
			676	424	112	134	6			
1	D	86	Total	C	N	O	S	0	6	0
			703	440	116	142	5			

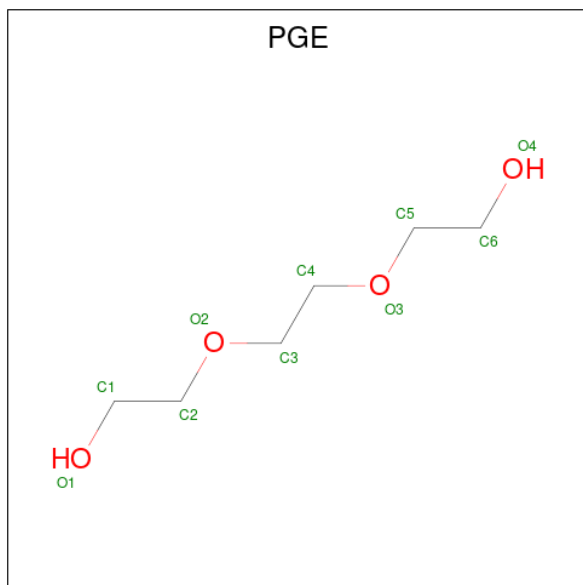
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	expression tag	UNP Q96CV9
A	418	PRO	-	expression tag	UNP Q96CV9
A	472	SER	CYS	engineered mutation	UNP Q96CV9
A	473	GLU	SER	engineered mutation	UNP Q96CV9
B	417	GLY	-	expression tag	UNP Q96CV9
B	418	PRO	-	expression tag	UNP Q96CV9
B	472	SER	CYS	engineered mutation	UNP Q96CV9
B	473	GLU	SER	engineered mutation	UNP Q96CV9
C	417	GLY	-	expression tag	UNP Q96CV9
C	418	PRO	-	expression tag	UNP Q96CV9
C	472	SER	CYS	engineered mutation	UNP Q96CV9
C	473	GLU	SER	engineered mutation	UNP Q96CV9
D	417	GLY	-	expression tag	UNP Q96CV9
D	418	PRO	-	expression tag	UNP Q96CV9
D	472	SER	CYS	engineered mutation	UNP Q96CV9
D	473	GLU	SER	engineered mutation	UNP Q96CV9

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RNF31.

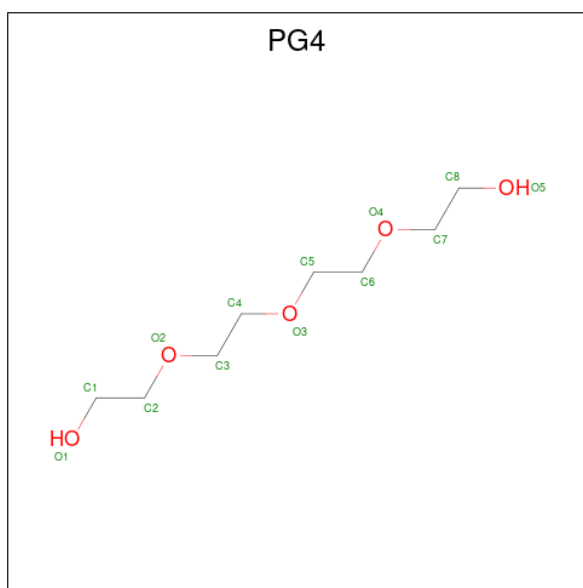
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	29	Total	C	N	O	S	0	2	0
			230	139	44	43	4			
2	E	29	Total	C	N	O	S	0	3	0
			239	145	44	46	4			

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			6	4	2		
3	G	1	Total	C	O	0	0
			9	6	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			6	4	2		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			8	5	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		
6	B	57	Total	O	0	0
			57	57		
6	G	37	Total	O	0	0
			37	37		
6	C	52	Total	O	0	0
			52	52		
6	D	59	Total	O	0	0
			59	59		

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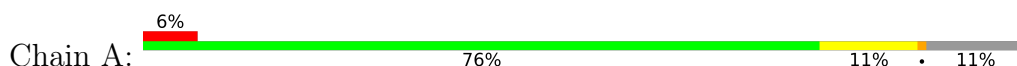
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	29	Total	O	0	0
			29	29		

3 Residue-property plots [i](#)

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: Optineurin



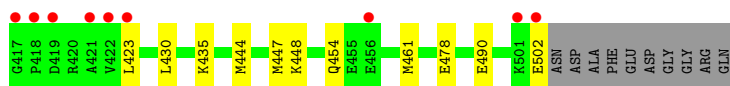
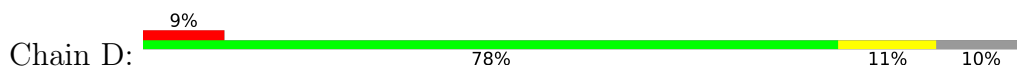
- Molecule 1: Optineurin



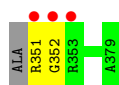
- Molecule 1: Optineurin



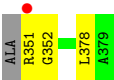
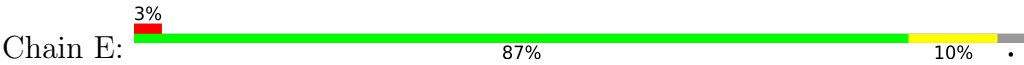
- Molecule 1: Optineurin



- Molecule 2: E3 ubiquitin-protein ligase RNF31



- Molecule 2: E3 ubiquitin-protein ligase RNF31



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.76Å 92.68Å 149.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.27 – 1.70 58.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.27-1.70) 100.0 (58.27-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.196 , 0.222 0.201 , 0.225	Depositor DCC
R_{free} test set	3985 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3638	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% 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: ZN, PG4, PGE

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	0.59	1/722 (0.1%)	0.65	0/962
1	B	0.76	1/717 (0.1%)	0.98	6/957 (0.6%)
1	C	0.70	1/691 (0.1%)	0.87	4/922 (0.4%)
1	D	0.68	0/725	0.76	0/971
2	E	0.77	0/254	0.85	0/340
2	G	0.82	0/239	0.83	0/320
All	All	0.70	3/3348 (0.1%)	0.82	10/4472 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	468	MET	SD-CE	-6.36	1.63	1.79
1	C	456	GLU	CG-CD	6.12	1.67	1.52
1	A	447	MET	SD-CE	-5.18	1.66	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	MET	CG-SD-CE	8.83	120.33	100.90
1	B	448	LYS	CG-CD-CE	8.66	131.21	111.30
1	C	456	GLU	CB-CG-CD	-7.80	99.34	112.60
1	C	456	GLU	CA-CB-CG	7.44	128.97	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	LYS	CA-CB-CG	6.61	127.31	114.10
1	B	425	GLU	N-CA-CB	-5.55	101.97	110.01
1	B	425	GLU	CB-CG-CD	5.28	121.58	112.60
1	C	456	GLU	CG-CD-OE2	5.24	130.46	118.40
1	C	422	VAL	CG1-CB-CG2	5.22	122.29	110.80
1	B	448	LYS	CB-CG-CD	-5.01	99.78	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	425	GLU	Sidechain

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	701	0	720	22	0
1	B	696	0	707	31	0
1	C	676	0	689	20	0
1	D	703	0	713	20	0
2	E	239	0	233	5	0
2	G	230	0	222	3	0
3	A	7	0	9	0	0
3	B	25	0	31	4	0
3	C	7	0	9	0	0
3	D	26	0	35	4	0
3	E	8	0	9	3	0
3	G	9	0	11	1	0
4	B	13	0	18	2	0
4	C	13	0	18	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	49	0	0	5	1
6	B	57	0	0	4	0
6	C	52	0	0	3	1
6	D	59	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	29	0	0	0	0
6	G	37	0	0	0	0
All	All	3638	0	3424	74	1

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 11.

All (74) 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:447:MET:HE3	1:B:447:MET:HE3	1.43	1.00
1:A:495:GLN:NE2	6:A:701:HOH:O	1.95	0.98
1:D:502:GLU:OE2	6:D:701:HOH:O	1.80	0.97
4:B:602:PG4:O5	6:B:701:HOH:O	1.83	0.95
1:D:490[B]:GLU:OE1	6:D:702:HOH:O	1.81	0.95
1:C:423:LEU:HD21	1:D:423:LEU:HD21	1.52	0.90
1:C:421:ALA:O	6:C:701:HOH:O	1.93	0.86
1:B:419:ASP:N	6:B:702:HOH:O	2.09	0.86
1:B:468:MET:HE2	1:B:471:TYR:HD2	1.41	0.85
2:G:351:ARG:HB2	3:G:402:PGE:H52	1.64	0.79
1:C:461:MET:HB2	1:D:461:MET:HE1	1.64	0.79
1:B:468:MET:HE2	1:B:471:TYR:CD2	2.17	0.79
1:A:447:MET:HE1	1:B:444:MET:HG2	1.68	0.76
1:A:473:GLU:OE1	6:A:702:HOH:O	2.05	0.75
1:A:462:THR:HA	1:B:461[B]:MET:HE2	1.70	0.73
1:C:444[B]:MET:HG3	1:D:447:MET:HE1	1.73	0.70
1:A:472[A]:SER:HB3	1:B:468:MET:HE1	1.72	0.70
2:G:351:ARG:HG3	2:G:352:GLY:O	1.91	0.70
3:B:601:PGE:O2	6:B:703:HOH:O	2.11	0.68
1:A:472[B]:SER:HB2	1:B:468:MET:HE1	1.75	0.67
1:A:420:ARG:N	6:A:703:HOH:O	2.27	0.67
1:A:447:MET:CE	1:B:444:MET:HG2	2.25	0.66
1:D:448:LYS:HG3	3:D:602:PGE:H2	1.77	0.64
1:B:465:ARG:NH2	1:B:469[A]:GLU:OE1	2.25	0.63
1:A:441:GLN:HE21	1:B:440:LYS:HZ1	1.47	0.62
1:A:447:MET:HE3	1:B:447:MET:CE	2.25	0.61
1:A:420:ARG:N	6:A:705:HOH:O	2.32	0.61
2:E:351:ARG:HE	3:E:402:PGE:C2	2.14	0.61
3:D:603:PGE:H22	2:E:378:LEU:HB3	1.81	0.60
2:E:351:ARG:HB2	3:E:402:PGE:O2	2.02	0.60
1:B:459[B]:GLU:HG3	1:B:460:THR:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:LYS:NZ	3:D:603:PGE:O4	2.27	0.59
1:C:447:MET:SD	1:D:444[A]:MET:HG3	2.43	0.59
1:B:429:LYS:HG3	3:B:604:PGE:H42	1.87	0.57
1:C:423:LEU:HD22	1:D:423:LEU:HD11	1.86	0.57
1:B:468:MET:CE	1:B:471:TYR:CD2	2.87	0.56
1:A:447:MET:HE1	1:B:444:MET:CG	2.34	0.56
1:C:459:GLU:HA	1:C:462:THR:HG22	1.87	0.56
1:A:441:GLN:NE2	1:B:440:LYS:NZ	2.54	0.55
1:A:441:GLN:HE21	1:B:440:LYS:NZ	2.04	0.55
1:A:447:MET:HE1	1:B:444:MET:CB	2.37	0.55
1:C:454:GLN:NE2	1:D:454:GLN:OE1	2.39	0.54
1:B:422:VAL:O	1:B:425:GLU:HB2	2.08	0.53
1:B:459[B]:GLU:HG3	1:B:460:THR:H	1.72	0.53
2:E:351:ARG:HG3	2:E:352:GLY:O	2.10	0.52
1:C:429:LYS:NZ	2:E:351:ARG:HG2	2.25	0.51
1:A:441:GLN:NE2	1:B:440:LYS:HZ1	2.08	0.51
1:C:421:ALA:HB1	6:C:701:HOH:O	2.11	0.51
1:A:435:LYS:NZ	6:A:706:HOH:O	2.43	0.50
1:A:444:MET:HG2	1:B:444:MET:HG2	1.94	0.50
1:D:435:LYS:HZ3	3:D:603:PGE:C1	2.25	0.49
1:D:502:GLU:CD	6:D:701:HOH:O	2.44	0.49
1:B:435:LYS:HE2	4:B:602:PG4:H11	1.93	0.49
1:C:435:LYS:NZ	6:C:704:HOH:O	2.43	0.48
1:B:422:VAL:HA	1:B:425:GLU:HG3	1.96	0.48
1:C:423:LEU:HD11	1:D:423:LEU:HD22	1.97	0.46
1:C:455[A]:GLU:HG2	1:D:454:GLN:HE22	1.81	0.46
1:C:455[A]:GLU:OE2	1:D:454:GLN:NE2	2.42	0.46
1:C:482:ARG:HD3	1:D:478:GLU:OE1	2.17	0.45
1:A:430:LEU:O	1:A:434:GLU:HG3	2.16	0.45
1:D:430:LEU:CD2	3:E:402:PGE:H3	2.47	0.45
1:B:456:GLU:O	1:B:459[B]:GLU:HG3	2.15	0.44
1:B:439:SER:HB3	3:B:603:PGE:H4	1.99	0.44
1:A:429:LYS:NZ	2:G:351:ARG:HG2	2.32	0.43
1:C:423:LEU:CD2	1:D:423:LEU:HD11	2.48	0.43
1:D:423:LEU:HD13	1:D:423:LEU:HA	1.64	0.43
1:B:435:LYS:HB3	1:B:435:LYS:HE3	1.91	0.43
1:B:495:GLN:OE1	6:B:705:HOH:O	2.20	0.43
1:C:479:ARG:HE	1:D:478:GLU:CD	2.27	0.43
1:C:460:THR:O	1:C:464:LEU:HD13	2.19	0.42
1:C:461:MET:HE3	1:C:465:ARG:HH12	1.83	0.42
1:B:429:LYS:HE3	3:B:604:PGE:H5	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:HG2	1:B:444:MET:CG	2.51	0.41
1:C:444[B]:MET:HE3	1:C:444[B]:MET:HB2	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:748:HOH:O	6:C:747:HOH:O[1_655]	2.12	0.08

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	89/96 (93%)	89 (100%)	0	0	100	100
1	B	87/96 (91%)	87 (100%)	0	0	100	100
1	C	85/96 (88%)	84 (99%)	1 (1%)	0	100	100
1	D	90/96 (94%)	90 (100%)	0	0	100	100
2	E	31/30 (103%)	31 (100%)	0	0	100	100
2	G	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
All	All	411/444 (93%)	409 (100%)	2 (0%)	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	75/81 (93%)	75 (100%)	0	100	100
1	B	74/81 (91%)	74 (100%)	0	100	100
1	C	71/81 (88%)	71 (100%)	0	100	100
1	D	75/81 (93%)	75 (100%)	0	100	100
2	E	27/23 (117%)	27 (100%)	0	100	100
2	G	25/23 (109%)	25 (100%)	0	100	100
All	All	347/370 (94%)	347 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	486	HIS
1	A	495	GLN
1	B	454	GLN
1	C	441	GLN
1	C	476	HIS
1	C	495	GLN
2	E	357	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	PGE	B	601	-	8,8,9	0.33	0	7,7,8	0.36	0
3	PGE	D	603	-	9,9,9	0.31	0	8,8,8	0.39	0
3	PGE	A	601	-	6,6,9	0.38	0	5,5,8	0.36	0
3	PGE	B	604	-	5,5,9	0.46	0	4,4,8	0.41	0
3	PGE	D	602	-	5,5,9	0.40	0	4,4,8	0.46	0
4	PG4	B	602	-	12,12,12	0.53	0	11,11,11	0.42	0
3	PGE	G	402	-	8,8,9	0.31	0	7,7,8	0.69	0
3	PGE	D	601	-	9,9,9	0.29	0	8,8,8	0.32	0
4	PG4	C	601	-	12,12,12	0.77	0	11,11,11	1.10	0
3	PGE	E	402	-	7,7,9	0.29	0	6,6,8	0.55	0
3	PGE	B	603	-	9,9,9	0.39	0	8,8,8	0.35	0
3	PGE	C	602	-	6,6,9	0.29	0	5,5,8	0.43	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
3	PGE	B	601	-	-	6/6/6/7	-
3	PGE	D	603	-	-	5/7/7/7	-
3	PGE	A	601	-	-	3/4/4/7	-
3	PGE	B	604	-	-	2/3/3/7	-
3	PGE	D	602	-	-	1/3/3/7	-
4	PG4	B	602	-	-	4/10/10/10	-
3	PGE	G	402	-	-	2/6/6/7	-
3	PGE	D	601	-	-	1/7/7/7	-
4	PG4	C	601	-	-	1/10/10/10	-
3	PGE	E	402	-	-	1/5/5/7	-
3	PGE	B	603	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	C	602	-	-	2/4/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	PGE	C1-C2-O2-C3
3	B	601	PGE	O2-C3-C4-O3
3	B	603	PGE	O2-C3-C4-O3
3	D	603	PGE	O1-C1-C2-O2
4	B	602	PG4	O1-C1-C2-O2
3	B	603	PGE	O1-C1-C2-O2
3	D	603	PGE	O2-C3-C4-O3
3	B	601	PGE	O3-C5-C6-O4
3	B	601	PGE	C4-C3-O2-C2
3	E	402	PGE	O2-C3-C4-O3
3	B	603	PGE	O3-C5-C6-O4
3	C	602	PGE	O2-C3-C4-O3
4	C	601	PG4	O3-C5-C6-O4
3	A	601	PGE	O2-C3-C4-O3
3	B	601	PGE	C1-C2-O2-C3
3	B	601	PGE	C6-C5-O3-C4
4	B	602	PG4	C5-C6-O4-C7
3	D	601	PGE	C1-C2-O2-C3
4	B	602	PG4	C3-C4-O3-C5
3	B	601	PGE	C3-C4-O3-C5
3	B	603	PGE	C4-C3-O2-C2
3	B	603	PGE	C6-C5-O3-C4
3	D	603	PGE	C3-C4-O3-C5
3	D	603	PGE	C1-C2-O2-C3
3	A	601	PGE	O1-C1-C2-O2
3	G	402	PGE	C1-C2-O2-C3
3	B	603	PGE	C3-C4-O3-C5
3	B	604	PGE	C6-C5-O3-C4
3	G	402	PGE	C3-C4-O3-C5
3	D	602	PGE	C4-C3-O2-C2
3	B	604	PGE	O2-C3-C4-O3
3	D	603	PGE	O3-C5-C6-O4
4	B	602	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
3	C	602	PGE	C1-C2-O2-C3

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	PGE	1	0
3	D	603	PGE	3	0
3	B	604	PGE	2	0
3	D	602	PGE	1	0
4	B	602	PG4	2	0
3	G	402	PGE	1	0
3	E	402	PGE	3	0
3	B	603	PGE	1	0

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	85/96 (88%)	0.50	6 (7%)	22 24	15, 33, 62, 76	6 (7%)
1	B	83/96 (86%)	0.69	11 (13%)	7 6	16, 27, 66, 84	6 (7%)
1	C	83/96 (86%)	0.99	13 (15%)	5 4	16, 33, 59, 79	4 (4%)
1	D	86/96 (89%)	0.66	9 (10%)	11 11	14, 29, 55, 90	6 (6%)
2	E	29/30 (96%)	-0.11	1 (3%)	48 52	10, 22, 46, 71	3 (10%)
2	G	29/30 (96%)	-0.09	3 (10%)	12 12	14, 21, 55, 72	2 (6%)
All	All	395/444 (88%)	0.59	43 (10%)	10 10	10, 29, 63, 90	27 (6%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ALA	8.1
1	C	463	ILE	7.3
1	D	417	GLY	6.9
1	D	419	ASP	6.7
1	C	502	GLU	6.2
1	B	420	ARG	6.2
1	B	422	VAL	5.6
1	A	422	VAL	5.2
1	C	420	ARG	5.1
1	C	462	THR	4.8
1	D	418	PRO	4.8
1	A	504	ASP	4.8
1	D	502	GLU	4.7
1	C	423	LEU	4.4
1	D	423	LEU	4.3
1	B	423	LEU	4.2
1	C	422	VAL	3.9
1	A	421	ALA	3.9
1	C	460	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	424	LYS	3.8
1	C	466	ALA	3.7
1	A	420	ARG	3.6
1	C	464	LEU	3.5
1	D	422	VAL	3.5
1	B	419	ASP	3.4
1	B	425	GLU	3.4
2	E	351	ARG	3.4
1	C	467	GLN	3.3
1	A	503	ASN	3.3
2	G	351	ARG	3.1
1	C	421	ALA	3.1
1	A	423	LEU	3.0
1	B	426	LEU	2.8
1	D	456	GLU	2.6
2	G	352	GLY	2.5
1	C	459	GLU	2.4
1	C	456	GLU	2.4
1	D	421	ALA	2.3
1	D	501	LYS	2.2
2	G	353	ARG	2.2
1	B	501	LYS	2.1
1	B	427	SER	2.1
1	B	448	LYS	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($\text{\AA}^2$)	Q<0.9
3	PGE	D	602	6/10	0.73	0.29	65,69,70,71	0
4	PG4	C	601	13/13	0.75	0.26	42,51,67,72	0
3	PGE	B	603	10/10	0.78	0.25	57,68,74,74	0
3	PGE	D	603	10/10	0.80	0.30	82,88,96,97	0
4	PG4	B	602	13/13	0.82	0.22	60,66,76,82	0
3	PGE	E	402	8/10	0.83	0.30	70,77,83,84	0
3	PGE	A	601	7/10	0.83	0.21	64,65,65,66	0
3	PGE	B	604	6/10	0.83	0.25	54,56,61,62	0
3	PGE	C	602	7/10	0.84	0.23	78,80,83,86	0
3	PGE	B	601	9/10	0.86	0.21	58,69,75,75	0
3	PGE	G	402	9/10	0.86	0.26	66,74,81,82	0
3	PGE	D	601	10/10	0.91	0.14	37,42,50,54	0
5	ZN	G	401	1/1	0.99	0.03	17,17,17,17	0
5	ZN	E	401	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.