



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 AM UTC

PDB ID : 4N3Z / pdb_00004n3z
Title : Crystal structure of Rabex-5delta and Rabaptin-5C21 complex
Authors : Zhang, Z.; Zhang, T.; Ding, J.
Deposited on : 2013-10-08
Resolution : 3.10 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

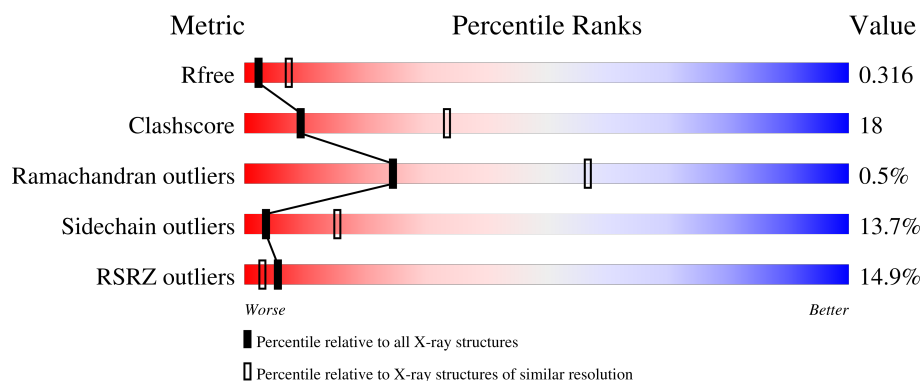
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	310	15% 43% 26% 7% 23%
2	B	92	3% 63% 22% • 11%
2	C	92	10% 54% 35% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3074 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 Rab5 GDP/GTP exchange factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1732	1084	307	329	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	expression tag	UNP Q9UJ41
A	125	GLY	-	expression tag	UNP Q9UJ41
A	126	HIS	-	expression tag	UNP Q9UJ41
A	127	HIS	-	expression tag	UNP Q9UJ41
A	128	HIS	-	expression tag	UNP Q9UJ41
A	129	HIS	-	expression tag	UNP Q9UJ41
A	130	HIS	-	expression tag	UNP Q9UJ41
A	131	HIS	-	expression tag	UNP Q9UJ41
A	?	-	GLY	deletion	UNP Q9UJ41
A	?	-	GLN	deletion	UNP Q9UJ41
A	?	-	THR	deletion	UNP Q9UJ41
A	?	-	SER	deletion	UNP Q9UJ41
A	?	-	PRO	deletion	UNP Q9UJ41
A	?	-	ARG	deletion	UNP Q9UJ41
A	?	-	LYS	deletion	UNP Q9UJ41
A	?	-	GLN	deletion	UNP Q9UJ41
A	?	-	GLU	deletion	UNP Q9UJ41
A	?	-	ALA	deletion	UNP Q9UJ41
A	?	-	GLU	deletion	UNP Q9UJ41
A	?	-	SER	deletion	UNP Q9UJ41
A	?	-	TRP	deletion	UNP Q9UJ41
A	?	-	SER	deletion	UNP Q9UJ41
A	?	-	PRO	deletion	UNP Q9UJ41
A	?	-	ASP	deletion	UNP Q9UJ41
A	?	-	ALA	deletion	UNP Q9UJ41
A	?	-	CYS	deletion	UNP Q9UJ41
A	?	-	LEU	deletion	UNP Q9UJ41

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q9UJ41
A	?	-	VAL	deletion	UNP Q9UJ41
A	?	-	LYS	deletion	UNP Q9UJ41

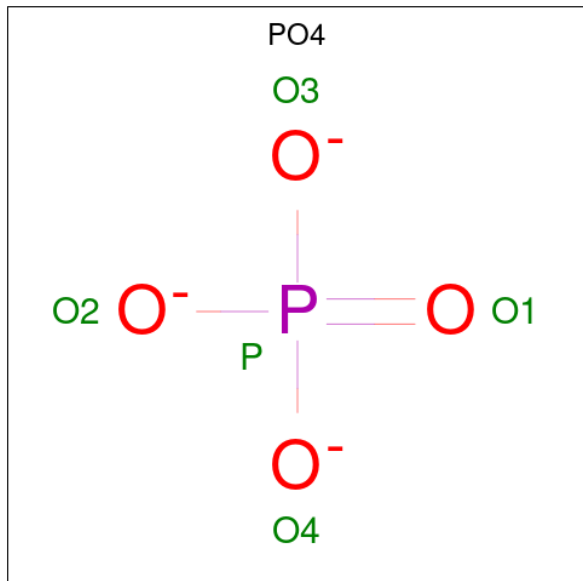
- Molecule 2 is a protein called Rab GTPase-binding effector protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			658	401	118	135	4			
2	C	83	Total	C	N	O	S	0	0	0
			669	407	122	136	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	551	MET	-	expression tag	UNP Q15276
C	551	MET	-	expression tag	UNP Q15276

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



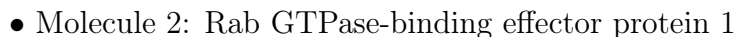
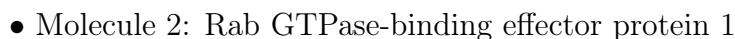
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 1: Rab5 GDP/GTP exchange factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.14Å 87.14Å 168.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.7 (50.00-3.10) 85.9 (50.00-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.43 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.264 , 0.315 0.264 , 0.316	Depositor DCC
R_{free} test set	601 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3074	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.45	0/1748	0.97	3/2365 (0.1%)
2	B	0.41	0/659	0.84	0/878
2	C	0.45	0/670	0.80	0/892
All	All	0.44	0/3077	0.91	3/4135 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	LEU	N-CA-C	-7.11	104.64	113.38
1	A	342	CYS	N-CA-C	-7.11	95.66	110.80
1	A	271	ALA	N-CA-C	-5.63	105.23	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	0	1593	83	0
2	B	658	0	672	14	0
2	C	669	0	685	26	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
All	All	3074	0	2950	109	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 18.

All (109) 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:242:ILE:HG21	1:A:327:ASN:HD21	1.38	0.87
1:A:346:ARG:O	1:A:346:ARG:NH1	2.11	0.83
1:A:357:THR:HG22	2:C:598:ALA:HB1	1.67	0.76
1:A:405:ILE:HD11	2:C:606:SER:HB3	1.68	0.76
1:A:346:ARG:HH11	1:A:346:ARG:C	1.98	0.71
1:A:251:GLN:O	1:A:252:MET:HB3	1.89	0.70
1:A:346:ARG:HH21	1:A:352:ASP:N	1.89	0.70
2:C:554:ARG:NH1	2:C:555:ASP:OD1	2.26	0.69
2:B:571:LEU:HD13	2:C:571:LEU:HA	1.75	0.68
2:B:624:VAL:HG13	2:C:628:MET:HE2	1.75	0.68
1:A:395:LEU:O	1:A:399:ASN:ND2	2.25	0.68
1:A:347:LEU:HD11	2:C:602:ARG:HG2	1.78	0.66
2:B:593:SER:HA	2:B:595:GLN:HE22	1.60	0.65
1:A:421:ASP:O	1:A:425:ARG:N	2.29	0.65
2:B:595:GLN:H	2:B:595:GLN:CD	2.05	0.64
2:C:609:LEU:HD12	2:C:612:GLU:OE2	1.96	0.64
1:A:270:LYS:HA	1:A:273:THR:HB	1.80	0.64
2:B:553:THR:N	2:C:553:THR:HG21	2.12	0.64
1:A:320:ILE:O	1:A:324:LEU:N	2.28	0.63
1:A:427:VAL:HG12	1:A:428:GLN:HG3	1.78	0.63
1:A:346:ARG:NH2	1:A:353:GLY:H	1.97	0.62
1:A:423:ILE:HG21	2:C:624:VAL:HG13	1.81	0.62
1:A:346:ARG:NH2	1:A:352:ASP:OD2	2.32	0.61
1:A:279:ASP:HB3	1:A:329:PRO:HG2	1.84	0.60
2:C:623:ASP:HA	2:C:626:GLU:HG2	1.82	0.60
2:C:556:GLN:HA	2:C:559:LYS:HG2	1.84	0.59
1:A:351:GLU:O	1:A:354:TYR:N	2.36	0.59
2:B:613:LEU:HD21	2:C:614:GLN:HG2	1.85	0.59
2:C:596:ILE:HG22	2:C:599:LEU:H	1.68	0.58
1:A:250:PRO:HB3	1:A:255:VAL:HG13	1.85	0.58
2:C:591:ASP:H	2:C:595:GLN:HE22	1.51	0.58
1:A:251:GLN:O	1:A:252:MET:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HG23	1:A:328:PRO:HG3	1.86	0.57
1:A:404:ARG:HG2	1:A:405:ILE:N	2.20	0.56
1:A:283:VAL:HG12	1:A:285:ARG:H	1.71	0.56
1:A:398:LEU:HD12	2:B:600:VAL:HG12	1.88	0.56
1:A:235:ASP:OD2	1:A:333:SER:OG	2.25	0.55
2:C:618:SER:HA	2:C:621:LYS:HE2	1.88	0.54
1:A:249:THR:C	1:A:251:GLN:H	2.14	0.54
1:A:406:MET:O	1:A:410:LYS:HG2	2.07	0.53
1:A:291:ILE:HD11	1:A:359:LEU:HB2	1.89	0.53
1:A:288:LEU:O	1:A:292:THR:HG23	2.08	0.53
2:C:610:LEU:HD23	2:C:613:LEU:HD12	1.90	0.53
1:A:278:MET:HA	1:A:281:LYS:HD2	1.91	0.53
1:A:342:CYS:O	1:A:344:PRO:HD3	2.08	0.52
1:A:391:ASN:OD1	1:A:392:LEU:N	2.42	0.52
2:C:590:GLU:OE1	2:C:595:GLN:NE2	2.41	0.52
1:A:359:LEU:O	1:A:363:VAL:HG23	2.10	0.52
1:A:302:ILE:HG22	1:A:306:LYS:HE2	1.91	0.52
1:A:249:THR:O	1:A:251:GLN:N	2.40	0.51
1:A:429:ASP:OD1	1:A:430:ILE:HG13	2.10	0.51
1:A:429:ASP:OD1	1:A:430:ILE:N	2.40	0.51
1:A:270:LYS:HD2	1:A:297:HIS:CD2	2.45	0.51
1:A:330:ARG:O	1:A:334:ASN:ND2	2.33	0.50
1:A:266:ASP:O	1:A:270:LYS:HG2	2.12	0.50
1:A:284:PRO:HG2	1:A:341:PHE:O	2.12	0.49
2:B:588:SER:HB3	2:B:592:SER:HB3	1.92	0.49
2:B:554:ARG:HH12	2:C:553:THR:HA	1.78	0.48
1:A:401:ARG:O	1:A:405:ILE:HG23	2.13	0.48
1:A:318:THR:O	1:A:322:ILE:HG12	2.13	0.48
2:B:628:MET:HG2	2:B:632:MET:HE3	1.96	0.48
2:C:595:GLN:HG3	2:C:597:SER:N	2.29	0.47
1:A:277:GLU:CD	1:A:281:LYS:HZ2	2.22	0.47
1:A:289:ALA:O	1:A:293:LYS:HG2	2.14	0.47
1:A:237:ALA:HA	1:A:240:LYS:HE2	1.96	0.47
1:A:292:THR:OG1	1:A:293:LYS:N	2.48	0.47
1:A:356:PHE:C	1:A:356:PHE:CD1	2.92	0.47
1:A:344:PRO:C	1:A:346:ARG:N	2.69	0.47
1:A:274:ASP:O	1:A:290:CYS:SG	2.73	0.46
1:A:277:GLU:CD	1:A:281:LYS:NZ	2.74	0.46
1:A:288:LEU:HA	1:A:291:ILE:HG22	1.98	0.46
1:A:261:ILE:HG12	1:A:264:VAL:HG13	1.99	0.45
1:A:319:LEU:O	1:A:323:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:PHE:CE1	1:A:360:CYS:SG	3.10	0.45
1:A:244:ALA:O	1:A:246:ARG:N	2.49	0.44
1:A:238:ILE:HD12	1:A:238:ILE:HA	1.88	0.44
1:A:354:TYR:O	1:A:358:ASN:ND2	2.44	0.44
1:A:396:SER:O	1:A:400:GLU:HG3	2.18	0.44
1:A:421:ASP:HB3	1:A:425:ARG:HG3	2.00	0.44
1:A:233:LYS:HG3	1:A:234:LYS:H	1.83	0.44
1:A:346:ARG:NH2	1:A:352:ASP:N	2.62	0.44
1:A:274:ASP:O	1:A:277:GLU:N	2.51	0.43
1:A:272:ILE:O	1:A:276:ILE:HG12	2.18	0.43
2:B:586:LYS:O	2:B:587:GLN:HB3	2.19	0.43
1:A:416:LEU:HD12	2:B:617:LEU:HD13	2.00	0.43
1:A:291:ILE:HD12	1:A:359:LEU:HD22	1.99	0.43
1:A:351:GLU:O	1:A:353:GLY:N	2.52	0.43
2:C:609:LEU:O	2:C:613:LEU:HG	2.19	0.42
1:A:357:THR:HG21	2:C:602:ARG:HG3	2.01	0.42
1:A:291:ILE:CD1	1:A:359:LEU:HD22	2.50	0.42
1:A:353:GLY:O	1:A:357:THR:HG23	2.20	0.42
2:C:591:ASP:H	2:C:595:GLN:NE2	2.15	0.42
1:A:249:THR:C	1:A:251:GLN:N	2.78	0.42
1:A:414:LYS:O	1:A:417:ILE:N	2.53	0.42
1:A:263:GLU:HG3	1:A:304:ILE:HD13	2.02	0.42
2:B:628:MET:HB2	2:C:628:MET:HE1	2.01	0.42
1:A:251:GLN:OE1	1:A:251:GLN:HA	2.17	0.41
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.90	0.41
1:A:245:LEU:HD12	1:A:366:ILE:HG23	2.02	0.41
2:B:599:LEU:HD21	2:C:600:VAL:HG22	2.01	0.41
1:A:263:GLU:CG	1:A:304:ILE:HD13	2.50	0.41
1:A:244:ALA:C	1:A:246:ARG:H	2.29	0.41
2:C:596:ILE:HG21	2:C:599:LEU:HG	2.03	0.41
1:A:285:ARG:HG3	1:A:286:ASP:N	2.36	0.40
1:A:243:ARG:O	1:A:246:ARG:HB3	2.21	0.40
1:A:245:LEU:HB2	1:A:324:LEU:HD11	2.02	0.40
1:A:278:MET:HG3	1:A:287:LYS:HB3	2.04	0.40
1:A:356:PHE:C	1:A:356:PHE:HD1	2.29	0.40
2:C:554:ARG:O	2:C:558:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	224/310 (72%)	200 (89%)	23 (10%)	1 (0%)	30	61
2	B	80/92 (87%)	76 (95%)	3 (4%)	1 (1%)	9	35
2	C	81/92 (88%)	75 (93%)	6 (7%)	0	100	100
All	All	385/494 (78%)	351 (91%)	32 (8%)	2 (0%)	24	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
2	B	587	GLN

5.3.2 Protein sidechains

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	164/288 (57%)	138 (84%)	26 (16%)	2	12
2	B	75/85 (88%)	64 (85%)	11 (15%)	3	14
2	C	76/85 (89%)	70 (92%)	6 (8%)	11	37
All	All	315/458 (69%)	272 (86%)	43 (14%)	3	15

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ASP

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Mol	Chain	Res	Type
1	A	238	ILE
1	A	246	ARG
1	A	251	GLN
1	A	255	VAL
1	A	261	ILE
1	A	264	VAL
1	A	280	SER
1	A	282	ARG
1	A	285	ARG
1	A	320	ILE
1	A	323	VAL
1	A	327	ASN
1	A	333	SER
1	A	335	ILE
1	A	351	GLU
1	A	352	ASP
1	A	363	VAL
1	A	367	GLU
1	A	397	GLN
1	A	401	ARG
1	A	404	ARG
1	A	423	ILE
1	A	426	GLU
1	A	427	VAL
1	A	430	ILE
2	B	553	THR
2	B	569	ASP
2	B	579	GLN
2	B	590	GLU
2	B	591	ASP
2	B	594	HIS
2	B	595	GLN
2	B	600	VAL
2	B	606	SER
2	B	611	GLU
2	B	633	GLN
2	C	554	ARG
2	C	569	ASP
2	C	572	GLU
2	C	601	LEU
2	C	630	VAL
2	C	633	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	397	GLN
2	B	587	GLN
2	B	595	GLN
2	B	627	GLN
2	C	561	GLN
2	C	594	HIS
2	C	595	GLN
2	C	625	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 oligosaccharides 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	$\# Z > 2$
3	PO4	C	701	-	4,4,4	0.89	0	6,6,6	0.66	0
3	PO4	A	501	-	4,4,4	1.01	0	6,6,6	0.40	0
3	PO4	B	701	-	4,4,4	0.96	0	6,6,6	0.52	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	238/310 (76%)	1.07	48 (20%) 3 1	23, 75, 144, 226	0
2	B	82/92 (89%)	0.28	3 (3%) 45 25	31, 58, 101, 134	0
2	C	83/92 (90%)	0.59	9 (10%) 11 6	19, 55, 103, 126	0
All	All	403/494 (81%)	0.81	60 (14%) 5 3	19, 65, 135, 226	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	PHE	6.6
1	A	186	TYR	6.6
1	A	188	ASN	5.9
1	A	216	MET	4.5
1	A	206	LYS	4.4
1	A	214	TYR	4.2
1	A	178	GLN	4.2
1	A	171	ARG	4.0
1	A	283	VAL	3.8
1	A	329	PRO	3.7
1	A	148	THR	3.7
1	A	209	ASP	3.5
1	A	252	MET	3.5
1	A	427	VAL	3.4
1	A	183	GLN	3.2
2	C	604	GLN	3.1
1	A	169	TYR	3.1
1	A	141	GLU	3.1
1	A	215	ILE	3.0
1	A	327	ASN	3.0
1	A	160	THR	2.9
1	A	425	ARG	2.9
1	A	350	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	346	ARG	2.8
1	A	184	ASP	2.7
1	A	145	PHE	2.7
2	C	594	HIS	2.7
2	C	630	VAL	2.7
1	A	338	ILE	2.6
1	A	251	GLN	2.6
1	A	266	ASP	2.6
2	C	553	THR	2.5
1	A	422	GLY	2.5
1	A	217	THR	2.5
1	A	271	ALA	2.4
1	A	165	GLU	2.4
1	A	235	ASP	2.4
2	B	589	SER	2.3
2	B	555	ASP	2.3
1	A	167	MET	2.3
1	A	426	GLU	2.3
2	C	595	GLN	2.3
1	A	429	ASP	2.3
2	C	587	GLN	2.2
1	A	176	GLU	2.2
1	A	173	LEU	2.2
1	A	179	SER	2.2
1	A	218	ARG	2.2
2	B	561	GLN	2.2
1	A	142	PHE	2.2
1	A	207	ILE	2.1
1	A	344	PRO	2.1
1	A	175	ILE	2.1
1	A	189	VAL	2.1
1	A	279	ASP	2.1
2	C	612	GLU	2.1
1	A	247	TRP	2.1
2	C	572	GLU	2.1
2	C	592	SER	2.0
1	A	421	ASP	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 [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	PO4	B	701	5/5	0.56	0.15	134,134,135,141	0
3	PO4	A	501	5/5	0.79	0.14	112,116,118,122	0
3	PO4	C	701	5/5	0.90	0.15	96,98,101,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.