



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:41 PM EDT

PDB ID : 3TEQ / pdb_00003teq
Title : Crystal structure of SOAR domain
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Deposited on : 2011-08-15
Resolution : 1.90 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

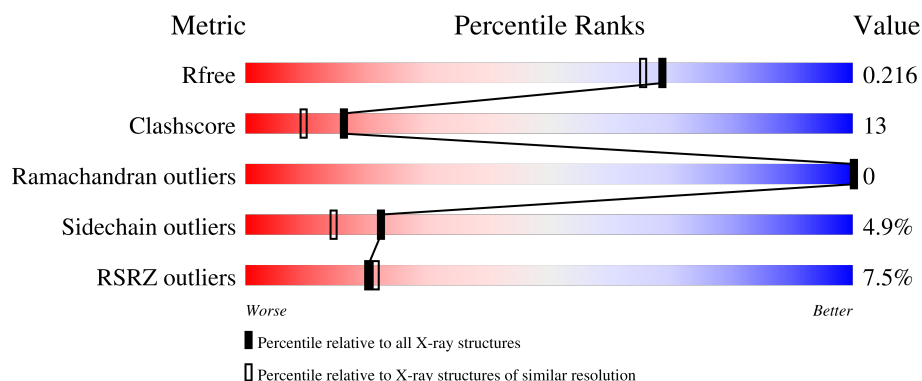
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	101	9% 73% 25% ..
1	B	101	2% 75% 23% .
1	C	101	5% 70% 27% .
1	D	101	14% 67% 26% 5% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	5	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3886 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.

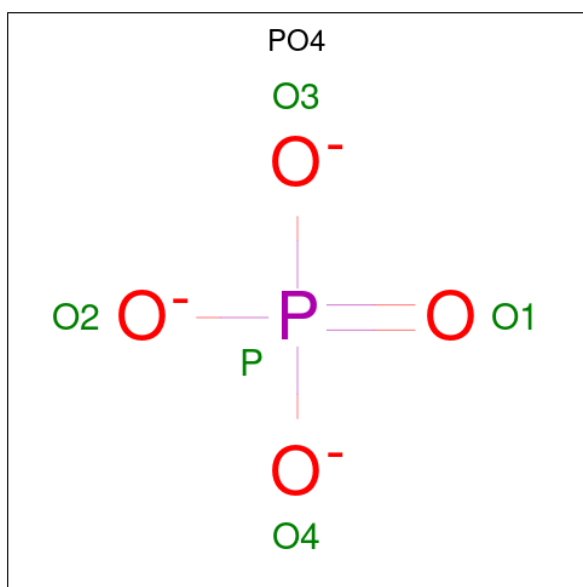
- Molecule 1 is a protein called Stromal interaction molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			815	517	148	149	1			
1	B	101	Total	C	N	O	S	0	0	0
			824	521	150	152	1			
1	C	101	Total	C	N	O	S	0	0	0
			824	521	150	152	1			
1	D	100	Total	C	N	O	S	0	0	0
			815	517	148	149	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	MET	LEU	engineered mutation	UNP Q13586
A	419	ALA	VAL	engineered mutation	UNP Q13586
A	437	THR	CYS	engineered mutation	UNP Q13586
B	374	MET	LEU	engineered mutation	UNP Q13586
B	419	ALA	VAL	engineered mutation	UNP Q13586
B	437	THR	CYS	engineered mutation	UNP Q13586
C	374	MET	LEU	engineered mutation	UNP Q13586
C	419	ALA	VAL	engineered mutation	UNP Q13586
C	437	THR	CYS	engineered mutation	UNP Q13586
D	374	MET	LEU	engineered mutation	UNP Q13586
D	419	ALA	VAL	engineered mutation	UNP Q13586
D	437	THR	CYS	engineered mutation	UNP Q13586

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

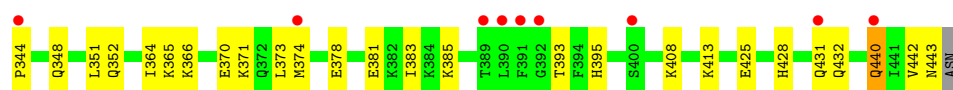
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total	O	0	0
			151	151		
3	B	157	Total	O	0	0
			157	157		
3	C	145	Total	O	0	0
			145	145		
3	D	130	Total	O	0	0
			130	130		

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: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



- Molecule 1: Stromal interaction molecule 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.58Å 90.58Å 104.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.20 – 1.90 25.20 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.20-1.90) 99.5 (25.20-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 1.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.249 0.221 , 0.216	Depositor DCC
R_{free} test set	1978 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4406e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.47	0/828	0.98	4/1113 (0.4%)
1	B	0.49	0/837	0.93	3/1124 (0.3%)
1	C	0.59	0/837	0.98	3/1124 (0.3%)
1	D	0.59	0/828	1.12	8/1113 (0.7%)
All	All	0.54	0/3330	1.00	18/4474 (0.4%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	VAL	N-CA-C	10.72	120.50	110.74
1	D	393	THR	N-CA-C	9.23	121.42	111.36
1	D	419	ALA	N-CA-C	-7.06	103.59	111.28
1	D	442	VAL	CB-CA-C	-6.84	103.26	111.81
1	B	440	GLN	N-CA-C	-6.77	98.20	108.96
1	B	344	PRO	N-CA-CB	6.71	110.39	103.00
1	A	440	GLN	N-CA-C	-6.66	97.88	108.73
1	D	344	PRO	N-CA-CB	6.34	109.97	103.00
1	A	344	PRO	N-CA-CB	6.20	109.82	103.00
1	C	344	PRO	N-CA-CB	5.58	109.14	103.00
1	D	440	GLN	N-CA-C	-5.58	99.64	108.73
1	A	393	THR	N-CA-C	5.55	117.41	111.36
1	D	442	VAL	CA-C-N	-5.50	111.80	121.70
1	D	442	VAL	C-N-CA	-5.50	111.80	121.70
1	C	440	GLN	N-CA-C	-5.13	100.15	108.41
1	D	442	VAL	N-CA-CB	5.12	116.20	110.62
1	B	400	SER	N-CA-C	5.05	117.52	111.71
1	C	441	ILE	N-CA-C	5.03	115.98	111.90

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	815	0	829	25	1
1	B	824	0	835	21	0
1	C	824	0	835	25	1
1	D	815	0	829	27	0
2	A	10	0	0	5	0
2	C	15	0	0	2	0
3	A	151	0	0	11	0
3	B	157	0	0	7	1
3	C	145	0	0	6	0
3	D	130	0	0	11	1
All	All	3886	0	3328	87	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 13.

All (87) 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:C:388:ASN:ND2	1:C:393:THR:HG22	1.60	1.15
1:D:371:LYS:HE3	3:D:567:HOH:O	1.48	1.13
1:D:365:LYS:HE2	3:D:292:HOH:O	1.64	0.97
1:C:388:ASN:HD21	1:C:393:THR:HG22	1.17	0.97
1:C:443:ASN:HB2	3:C:271:HOH:O	1.63	0.97
1:B:344:PRO:CB	3:B:100:HOH:O	2.18	0.91
1:A:364:ILE:HG13	3:A:492:HOH:O	1.71	0.89
1:C:345:GLU:HA	3:C:552:HOH:O	1.73	0.86
1:A:431:GLN:HB3	2:A:5:PO4:O1	1.77	0.84
1:C:428:HIS:ND1	1:D:407:HIS:HD2	1.74	0.83
1:C:349:LYS:NZ	2:C:6:PO4:O2	2.13	0.82
1:A:432:GLN:NE2	2:A:5:PO4:O4	2.12	0.81
1:D:440:GLN:NE2	3:D:123:HOH:O	2.00	0.80
1:B:403:ASP:OD2	3:B:478:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:HD2	3:B:585:HOH:O	1.85	0.75
1:A:431:GLN:NE2	2:A:5:PO4:O1	2.21	0.73
1:A:428:HIS:ND1	1:B:407:HIS:HD2	1.87	0.72
1:D:443:ASN:ND2	3:D:123:HOH:O	2.19	0.70
1:B:414:GLN:NE2	3:B:457:HOH:O	2.26	0.69
1:B:345:GLU:OE1	3:B:234:HOH:O	2.12	0.67
1:A:431:GLN:CB	2:A:5:PO4:O1	2.45	0.64
1:A:365:LYS:NZ	3:A:108:HOH:O	2.28	0.64
1:D:413:LYS:NZ	3:D:447:HOH:O	2.32	0.62
1:B:443:ASN:O	1:B:444:ASN:HB2	1.99	0.61
1:B:387:ARG:HD3	1:B:403:ASP:OD1	2.02	0.59
3:A:456:HOH:O	1:C:365:LYS:HE2	2.01	0.59
1:D:440:GLN:NE2	1:D:443:ASN:HB3	2.18	0.59
1:D:348:GLN:HE21	1:D:439:PHE:HB3	1.69	0.57
1:C:388:ASN:ND2	1:C:393:THR:CG2	2.53	0.57
1:A:364:ILE:HD13	3:A:189:HOH:O	2.04	0.57
1:D:365:LYS:NZ	3:D:463:HOH:O	2.37	0.57
1:C:372:GLN:NE2	3:C:452:HOH:O	2.34	0.56
1:C:344:PRO:HA	3:C:579:HOH:O	2.06	0.56
1:C:425:GLU:OE2	1:D:407:HIS:HE1	1.89	0.55
1:B:358:GLU:OE2	1:B:426:ARG:HG3	2.06	0.55
1:D:410:LEU:HG	3:D:57:HOH:O	2.05	0.55
1:A:425:GLU:OE2	1:B:407:HIS:HE1	1.89	0.54
1:A:364:ILE:CD1	3:A:189:HOH:O	2.58	0.52
1:A:381:GLU:HG2	1:A:385:LYS:HE3	1.92	0.52
1:D:386:LYS:HE2	3:D:505:HOH:O	2.10	0.51
1:C:394:PHE:O	1:C:398:HIS:HD2	1.93	0.51
1:A:381:GLU:O	1:A:385:LYS:HG3	2.10	0.51
1:B:394:PHE:O	1:B:398:HIS:HD2	1.93	0.51
1:A:413:LYS:NZ	3:A:529:HOH:O	2.36	0.50
1:A:408:LYS:HD3	3:A:322:HOH:O	2.10	0.50
1:A:371:LYS:HD2	3:A:599:HOH:O	2.10	0.50
1:B:352:GLN:O	1:B:356:GLU:HG3	2.12	0.50
1:B:396:VAL:HG12	3:B:447:HOH:O	2.12	0.50
1:C:442:VAL:CG1	1:C:443:ASN:N	2.74	0.50
1:B:378:GLU:HG2	1:B:382:LYS:HE3	1.94	0.49
1:D:414:GLN:O	1:D:417:SER:HB2	2.13	0.48
1:A:431:GLN:HE21	2:A:5:PO4:P	2.37	0.48
1:C:344:PRO:CA	3:C:579:HOH:O	2.61	0.48
1:D:398:HIS:CE1	3:D:228:HOH:O	2.66	0.48
1:D:358:GLU:OE2	1:D:426:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ASN:O	1:B:444:ASN:CB	2.61	0.48
1:A:425:GLU:OE2	1:B:407:HIS:CE1	2.67	0.48
1:C:428:HIS:ND1	1:D:407:HIS:CD2	2.66	0.47
1:A:443:ASN:OD1	3:A:601:HOH:O	2.21	0.47
1:D:374:MET:O	1:D:378:GLU:HG3	2.16	0.46
1:D:394:PHE:O	1:D:398:HIS:HD2	2.00	0.45
1:D:386:LYS:HB3	1:D:386:LYS:HE3	1.37	0.45
1:A:383:ILE:HD12	3:A:201:HOH:O	2.16	0.45
1:A:428:HIS:ND1	1:B:407:HIS:CD2	2.78	0.45
1:B:413:LYS:NZ	3:B:456:HOH:O	2.50	0.44
1:C:408:LYS:HB2	1:C:408:LYS:HE3	1.69	0.44
1:C:424:ARG:HG2	1:D:405:VAL:CG1	2.47	0.44
1:C:413:LYS:HB3	2:C:1:PO4:O3	2.17	0.43
1:D:427:LEU:O	1:D:431:GLN:HG3	2.19	0.43
1:B:383:ILE:O	1:B:387:ARG:HG3	2.19	0.43
1:C:425:GLU:OE2	1:D:407:HIS:CE1	2.69	0.43
1:C:414:GLN:OE1	3:C:558:HOH:O	2.21	0.43
1:C:347:LEU:HG	1:C:351:LEU:HD22	2.01	0.43
1:B:400:SER:H	1:C:360:GLN:HE22	1.67	0.42
1:D:391:PHE:HB3	1:D:395:HIS:CD2	2.54	0.42
1:A:348:GLN:O	1:A:352:GLN:HG3	2.19	0.42
1:A:395:HIS:CE1	3:A:527:HOH:O	2.72	0.41
1:C:423:LEU:O	1:C:427:LEU:HG	2.20	0.41
1:D:427:LEU:HD12	3:D:320:HOH:O	2.19	0.41
1:A:425:GLU:HG2	1:B:407:HIS:CE1	2.56	0.41
1:D:344:PRO:N	3:D:19:HOH:O	2.53	0.41
1:D:428:HIS:O	1:D:432:GLN:HG2	2.20	0.41
1:A:374:MET:O	1:A:378:GLU:HG3	2.20	0.41
1:D:348:GLN:O	1:D:352:GLN:HG3	2.21	0.41
1:C:385:LYS:O	1:C:389:THR:HG23	2.21	0.41
1:C:442:VAL:HG12	1:C:443:ASN:N	2.36	0.40
1:A:366:LYS:O	1:A:370:GLU:HG3	2.22	0.40

All (2) 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)
1:C:431:GLN:NE2	3:B:487:HOH:O[6_554]	2.09	0.11
1:A:440:GLN:OE1	3:D:453:HOH:O[5_544]	2.15	0.05

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	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
1	B	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
1	C	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
1	D	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
All	All	394/404 (98%)	384 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	86/88 (98%)	84 (98%)	2 (2%)	44	40
1	B	87/88 (99%)	84 (97%)	3 (3%)	32	25
1	C	87/88 (99%)	82 (94%)	5 (6%)	18	11
1	D	86/88 (98%)	79 (92%)	7 (8%)	11	5
All	All	346/352 (98%)	329 (95%)	17 (5%)	22	14

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	LEU
1	A	373	LEU

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Mol	Chain	Res	Type
1	B	351	LEU
1	B	373	LEU
1	B	386	LYS
1	C	351	LEU
1	C	373	LEU
1	C	381	GLU
1	C	388	ASN
1	C	416	LEU
1	D	351	LEU
1	D	371	LYS
1	D	386	LYS
1	D	414	GLN
1	D	416	LEU
1	D	417	SER
1	D	440	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	367	GLN
1	A	398	HIS
1	A	414	GLN
1	A	431	GLN
1	A	440	GLN
1	B	398	HIS
1	B	407	HIS
1	C	352	GLN
1	C	360	GLN
1	C	372	GLN
1	C	388	ASN
1	C	398	HIS
1	C	431	GLN
1	C	440	GLN
1	D	348	GLN
1	D	367	GLN
1	D	398	HIS
1	D	407	HIS
1	D	432	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	2	-	4,4,4	1.84	1 (25%)	6,6,6	0.47	0
2	PO4	C	1	-	4,4,4	1.72	1 (25%)	6,6,6	0.57	0
2	PO4	C	6	-	4,4,4	2.14	1 (25%)	6,6,6	0.36	0
2	PO4	A	5	-	4,4,4	1.43	0	6,6,6	1.07	0
2	PO4	C	4	-	4,4,4	1.97	1 (25%)	6,6,6	0.47	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	PO4	P-O1	3.63	1.59	1.50
2	C	4	PO4	P-O1	3.26	1.58	1.50
2	A	2	PO4	P-O1	3.15	1.57	1.50
2	C	1	PO4	P-O1	2.77	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	PO4	1	0
2	C	6	PO4	1	0
2	A	5	PO4	5	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	100/101 (99%)	0.46	9 (9%) 15 16	13, 26, 40, 44	0
1	B	101/101 (100%)	0.25	2 (1%) 65 69	14, 22, 34, 42	0
1	C	101/101 (100%)	0.38	5 (4%) 34 36	14, 24, 35, 42	0
1	D	100/101 (99%)	0.66	14 (14%) 6 6	16, 27, 39, 48	0
All	All	402/404 (99%)	0.44	30 (7%) 20 21	13, 25, 38, 48	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	PRO	7.2
1	D	443	ASN	5.1
1	D	391	PHE	4.0
1	D	390	LEU	3.8
1	D	392	GLY	3.5
1	D	419	ALA	3.4
1	C	443	ASN	3.4
1	A	392	GLY	3.2
1	D	388	ASN	3.1
1	C	419	ALA	2.8
1	A	344	PRO	2.8
1	D	417	SER	2.8
1	D	345	GLU	2.8
1	D	389	THR	2.8
1	D	442	VAL	2.8
1	A	440	GLN	2.6
1	A	389	THR	2.6
1	D	386	LYS	2.5
1	A	390	LEU	2.5
1	D	420	THR	2.4
1	D	374	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	393	THR	2.3
1	C	381	GLU	2.3
1	A	391	PHE	2.3
1	A	400	SER	2.2
1	B	381	GLU	2.2
1	C	417	SER	2.0
1	A	374	MET	2.0
1	A	431	GLN	2.0
1	C	344	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	C	6	5/5	0.56	0.15	73,74,74,74	0
2	PO4	C	4	5/5	0.68	0.15	82,82,83,83	0
2	PO4	A	5	5/5	0.69	0.15	67,68,69,69	0
2	PO4	A	2	5/5	0.76	0.18	80,80,81,81	0
2	PO4	C	1	5/5	0.77	0.13	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.