



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:15 PM UTC

PDB ID : 2UZQ / pdb_00002uzq
Title : Protein Phosphatase, New Crystal Form
Authors : Hillig, R.C.; Eberspaecher, U.
Deposited on : 2007-05-01
Resolution : 2.38 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

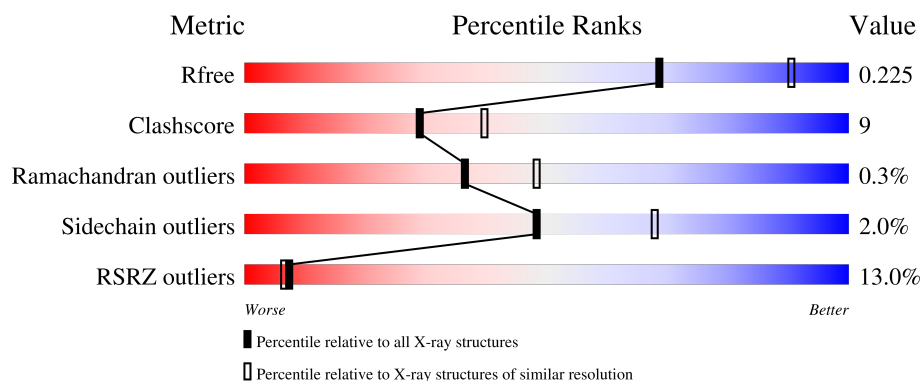
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	203	14% 67% 16% • 15%
1	B	203	14% 63% 20% • 15%
1	C	203	12% 67% 18% • 15%
1	D	203	9% 69% 14% • 15%
1	E	203	9% 66% 18% • 15%

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Mol	Chain	Length	Quality of chain
1	F	203	8% 68% 16% 15%

2 Entry composition [i](#)

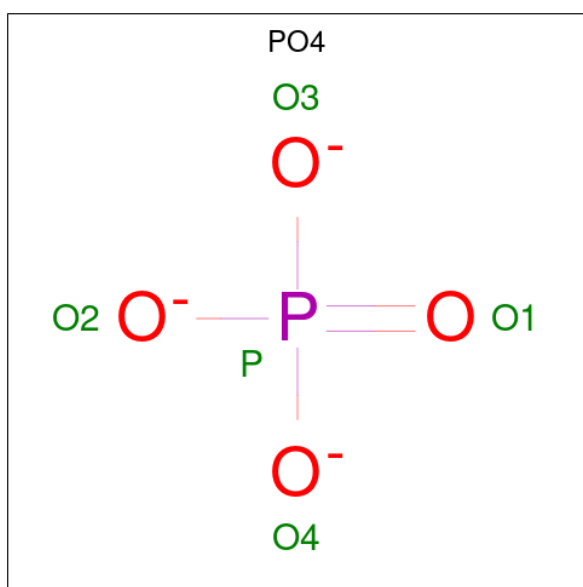
There are 3 unique types of molecules in this entry. The entry contains 8698 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 M-PHASE INDUCER PHOSPHATASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			
1	B	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			
1	C	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			
1	D	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			
1	E	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			
1	F	172	Total	C	N	O	S	0	0	1
			1412	912	236	255	9			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

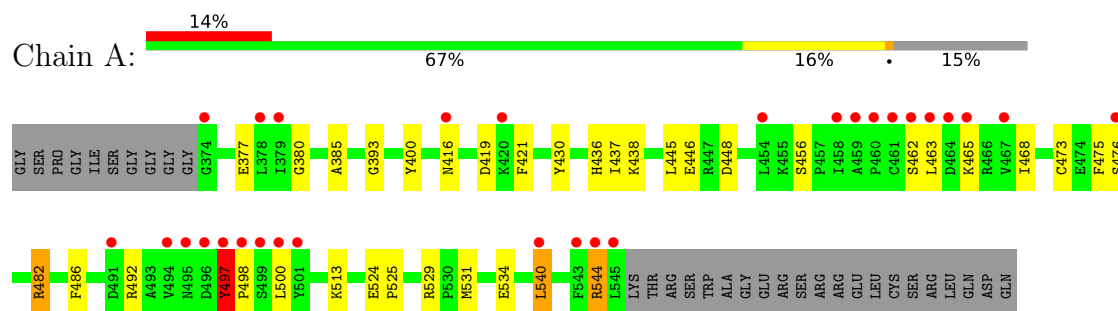
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	26	Total O 26 26	0	0
3	C	40	Total O 40 40	0	0
3	D	44	Total O 44 44	0	0
3	E	30	Total O 30 30	0	0
3	F	29	Total O 29 29	0	0

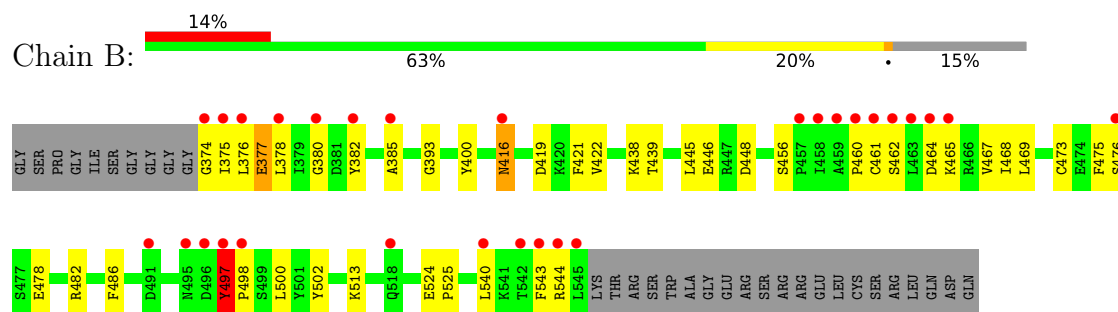
3 Residue-property plots

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.

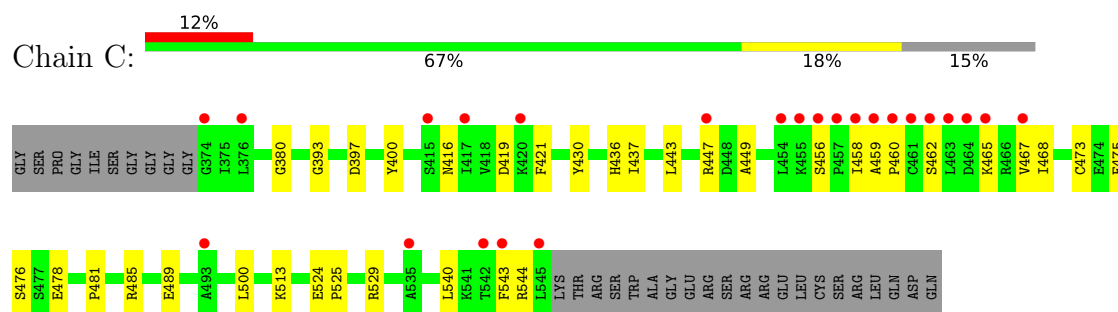
• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2



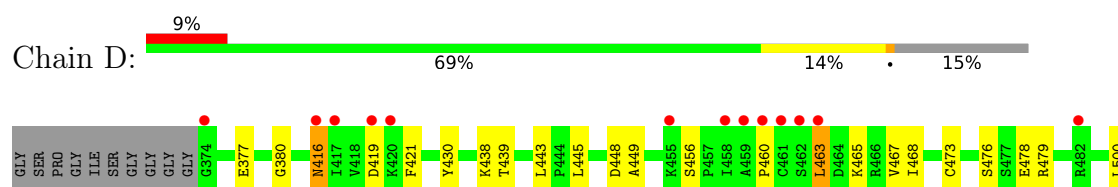
• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2

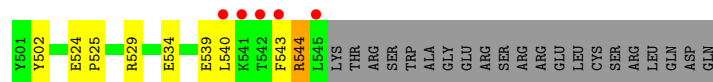


• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2

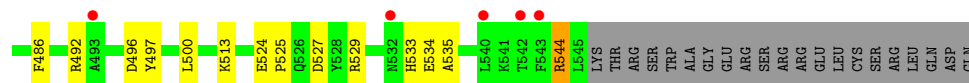


• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2

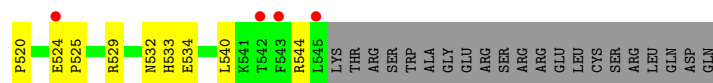
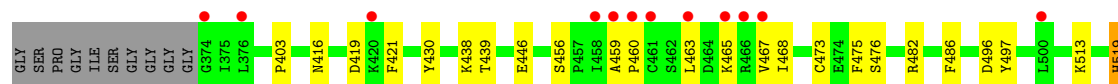




• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2



• Molecule 1: M-PHASE INDUCER PHOSPHATASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	123.92Å 123.92Å 174.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.77 – 2.38 36.77 – 2.38	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.77-2.38) 97.7 (36.77-2.38)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.39Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.226 , 0.249 0.225 , 0.225	Depositor DCC
R_{free} test set	3142 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.80% 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	0.44	1/1451 (0.1%)	1.00	6/1959 (0.3%)
1	B	0.45	1/1451 (0.1%)	0.98	9/1959 (0.5%)
1	C	0.44	1/1451 (0.1%)	0.93	2/1959 (0.1%)
1	D	0.45	1/1451 (0.1%)	0.93	5/1959 (0.3%)
1	E	0.41	1/1451 (0.1%)	0.93	4/1959 (0.2%)
1	F	0.44	1/1451 (0.1%)	0.95	6/1959 (0.3%)
All	All	0.44	6/8706 (0.1%)	0.95	32/11754 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	544	ARG	C-N	-5.62	1.25	1.33
1	F	544	ARG	C-N	-5.58	1.25	1.33
1	B	544	ARG	C-N	-5.56	1.25	1.33
1	D	544	ARG	C-N	-5.53	1.25	1.33
1	E	544	ARG	C-N	-5.50	1.25	1.33
1	A	544	ARG	C-N	-5.46	1.25	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	TYR	CA-C-N	-10.19	107.70	119.32
1	A	497	TYR	C-N-CA	-10.19	107.70	119.32
1	A	497	TYR	N-CA-C	7.23	125.78	109.81
1	E	456	SER	CA-C-N	6.26	127.67	119.84
1	E	456	SER	C-N-CA	6.26	127.67	119.84
1	A	456	SER	CA-C-N	5.91	127.22	119.84
1	A	456	SER	C-N-CA	5.91	127.22	119.84
1	B	497	TYR	CA-C-N	-5.79	112.94	118.97
1	B	497	TYR	C-N-CA	-5.79	112.94	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	SER	CA-C-N	5.78	127.06	119.84
1	B	456	SER	C-N-CA	5.78	127.06	119.84
1	D	456	SER	CA-C-N	5.68	126.94	119.84
1	D	456	SER	C-N-CA	5.68	126.94	119.84
1	F	456	SER	CA-C-N	5.52	126.74	119.84
1	F	456	SER	C-N-CA	5.52	126.74	119.84
1	F	459	ALA	CA-C-N	5.51	125.42	119.85
1	F	459	ALA	C-N-CA	5.51	125.42	119.85
1	C	456	SER	CA-C-N	5.48	126.69	119.84
1	C	456	SER	C-N-CA	5.48	126.69	119.84
1	F	519	HIS	CA-C-N	5.46	125.54	119.32
1	F	519	HIS	C-N-CA	5.46	125.54	119.32
1	B	502	TYR	CA-C-N	5.42	125.03	119.56
1	B	502	TYR	C-N-CA	5.42	125.03	119.56
1	E	461	CYS	N-CA-C	-5.41	106.68	113.72
1	E	534	GLU	N-CA-C	5.38	117.14	111.28
1	D	534	GLU	N-CA-C	5.37	117.83	111.33
1	A	534	GLU	N-CA-C	5.30	117.74	111.33
1	B	461	CYS	N-CA-C	-5.20	106.88	113.18
1	B	497	TYR	N-CA-C	5.19	121.28	109.81
1	B	478	GLU	N-CA-C	5.06	118.87	111.34
1	D	502	TYR	CA-C-N	5.03	124.64	119.56
1	D	502	TYR	C-N-CA	5.03	124.64	119.56

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	1412	0	1386	25	0
1	B	1412	0	1386	32	1
1	C	1412	0	1386	25	0
1	D	1412	0	1386	18	0
1	E	1412	0	1386	28	0
1	F	1412	0	1386	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	27	0	0	0	0
3	B	26	0	0	0	0
3	C	40	0	0	0	0
3	D	44	0	0	0	0
3	E	30	0	0	1	0
3	F	29	0	0	1	0
All	All	8698	0	8316	146	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 9.

All (146) 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:482:ARG:HH11	1:A:482:ARG:HB3	1.24	0.99
1:B:460:PRO:HG3	1:B:467:VAL:HG23	1.49	0.94
1:E:460:PRO:HG3	1:E:467:VAL:HG23	1.50	0.92
1:A:482:ARG:HH11	1:A:482:ARG:CB	1.85	0.88
1:F:524:GLU:HA	1:F:525:PRO:C	2.00	0.86
1:F:460:PRO:HG3	1:F:467:VAL:HG23	1.58	0.86
1:B:419:ASP:HB2	1:B:465:LYS:HB2	1.61	0.82
1:A:482:ARG:HB3	1:A:482:ARG:NH1	1.93	0.82
1:B:416:ASN:HB2	1:E:461:CYS:HB2	1.63	0.80
1:F:419:ASP:HB2	1:F:465:LYS:HB3	1.64	0.78
1:B:419:ASP:HB2	1:B:465:LYS:CB	2.14	0.78
1:A:438:LYS:HG2	1:A:524:GLU:OE1	1.86	0.76
1:A:419:ASP:HB2	1:A:465:LYS:HB3	1.69	0.75
1:B:524:GLU:HA	1:B:525:PRO:C	2.11	0.74
1:B:497:TYR:HB3	1:B:498:PRO:HD3	1.71	0.73
1:A:524:GLU:HA	1:A:525:PRO:C	2.13	0.72
1:A:419:ASP:HB2	1:A:465:LYS:CB	2.19	0.71
1:B:438:LYS:HG2	1:B:524:GLU:OE1	1.89	0.71
1:F:419:ASP:HB2	1:F:465:LYS:CB	2.21	0.70
1:C:524:GLU:HA	1:C:525:PRO:C	2.17	0.70
1:E:419:ASP:HB2	1:E:465:LYS:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:GLU:HA	1:D:525:PRO:C	2.15	0.69
1:E:473:CYS:SG	1:E:476:SER:HA	2.35	0.66
1:B:460:PRO:HG3	1:B:467:VAL:CG2	2.25	0.66
1:E:524:GLU:HA	1:E:525:PRO:C	2.22	0.65
1:A:540:LEU:HD21	1:A:544:ARG:CZ	2.30	0.61
1:C:473:CYS:SG	1:C:476:SER:HA	2.42	0.59
1:F:460:PRO:HG3	1:F:467:VAL:CG2	2.31	0.59
1:D:478:GLU:HG3	1:D:479:ARG:N	2.18	0.59
1:C:460:PRO:HG3	1:C:467:VAL:HG23	1.85	0.58
1:D:473:CYS:SG	1:D:476:SER:HA	2.44	0.58
1:F:482:ARG:HH11	1:F:482:ARG:HG3	1.70	0.57
1:A:462:SER:HB3	1:A:465:LYS:HG3	1.86	0.56
1:B:473:CYS:SG	1:B:476:SER:HA	2.46	0.56
1:D:460:PRO:HG3	1:D:467:VAL:HG23	1.87	0.56
1:D:416:ASN:O	1:D:465:LYS:HE2	2.06	0.56
1:B:462:SER:HB3	1:B:465:LYS:HG3	1.89	0.55
1:E:460:PRO:HG3	1:E:467:VAL:CG2	2.32	0.55
1:B:462:SER:HB3	1:B:465:LYS:CG	2.37	0.55
1:B:475:PHE:CE1	1:B:513:LYS:HD3	2.42	0.55
1:E:475:PHE:CE1	1:E:513:LYS:HD3	2.42	0.55
1:A:473:CYS:SG	1:A:476:SER:HA	2.48	0.53
1:D:419:ASP:HB2	1:D:465:LYS:HB3	1.89	0.53
1:A:419:ASP:HB2	1:A:465:LYS:HB2	1.90	0.53
1:B:445:LEU:HB2	1:B:448:ASP:OD2	2.09	0.53
1:C:460:PRO:C	1:C:462:SER:H	2.17	0.53
1:A:497:TYR:HB3	1:A:498:PRO:HD3	1.90	0.53
1:B:377:GLU:O	1:B:385:ALA:HA	2.09	0.52
1:A:475:PHE:CE1	1:A:513:LYS:HD3	2.44	0.52
1:C:447:ARG:HH11	1:C:447:ARG:HG3	1.73	0.52
1:B:419:ASP:HB2	1:B:465:LYS:HB3	1.92	0.51
1:E:482:ARG:HB3	1:E:482:ARG:NH1	2.25	0.51
1:A:497:TYR:O	1:A:498:PRO:C	2.45	0.51
1:D:430:TYR:O	1:D:529:ARG:HD2	2.09	0.51
1:B:393:GLY:HA3	1:B:400:TYR:CD1	2.46	0.50
1:F:475:PHE:CE1	1:F:513:LYS:HD3	2.47	0.50
1:C:380:GLY:HA3	1:C:500:LEU:HD12	1.93	0.50
1:E:462:SER:HB3	1:E:465:LYS:CG	2.42	0.50
1:E:443:LEU:HD13	1:E:449:ALA:HA	1.94	0.49
1:B:462:SER:C	1:B:464:ASP:H	2.20	0.49
1:F:403:PRO:HG3	3:F:2021:HOH:O	2.13	0.49
1:F:430:TYR:O	1:F:529:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:C	1:B:540:LEU:HD23	2.38	0.48
1:E:393:GLY:HA3	1:E:400:TYR:CD1	2.48	0.48
1:E:447:ARG:HH11	1:E:447:ARG:HG3	1.77	0.48
1:E:462:SER:HB3	1:E:465:LYS:HG3	1.95	0.48
1:C:478:GLU:O	1:C:481:PRO:HD2	2.13	0.48
1:E:496:ASP:O	1:E:497:TYR:C	2.57	0.48
1:E:527:ASP:HB3	3:E:2026:HOH:O	2.13	0.48
1:D:445:LEU:HB2	1:D:448:ASP:OD2	2.13	0.48
1:B:380:GLY:HA3	1:B:500:LEU:HD12	1.96	0.47
1:C:475:PHE:CE1	1:C:513:LYS:HD3	2.49	0.47
1:E:492:ARG:HD3	1:E:500:LEU:HD21	1.96	0.47
1:F:473:CYS:SG	1:F:476:SER:HA	2.55	0.46
1:B:475:PHE:HE1	1:B:513:LYS:HD3	1.77	0.46
1:F:421:PHE:HA	1:F:468:ILE:O	2.16	0.46
1:B:374:GLY:C	1:B:376:LEU:H	2.24	0.46
1:E:475:PHE:HE1	1:E:513:LYS:HD3	1.81	0.46
1:C:393:GLY:HA3	1:C:400:TYR:CD1	2.51	0.46
1:C:447:ARG:HG3	1:C:447:ARG:NH1	2.31	0.45
1:A:540:LEU:HD21	1:A:544:ARG:NH2	2.31	0.45
1:D:380:GLY:HA3	1:D:500:LEU:HD12	1.98	0.45
1:A:531:MET:HG2	1:A:540:LEU:CD1	2.47	0.45
1:B:540:LEU:HD23	1:B:540:LEU:O	2.16	0.45
1:A:380:GLY:HA3	1:A:500:LEU:HD12	1.99	0.45
1:E:380:GLY:HA3	1:E:500:LEU:HD12	1.98	0.45
1:C:419:ASP:HB2	1:C:465:LYS:CB	2.47	0.45
1:C:421:PHE:HA	1:C:468:ILE:O	2.17	0.45
1:D:460:PRO:HG3	1:D:467:VAL:CG2	2.47	0.45
1:E:419:ASP:OD1	1:E:461:CYS:SG	2.66	0.45
1:E:421:PHE:HA	1:E:468:ILE:O	2.17	0.45
1:C:485:ARG:O	1:C:489:GLU:HG3	2.17	0.44
1:C:460:PRO:HG3	1:C:467:VAL:CG2	2.47	0.44
1:A:393:GLY:HA3	1:A:400:TYR:CD1	2.52	0.44
1:D:421:PHE:HA	1:D:468:ILE:O	2.16	0.44
1:E:446:GLU:HB3	1:E:486:PHE:CE2	2.53	0.44
1:B:446:GLU:HB3	1:B:486:PHE:CE2	2.52	0.44
1:C:397:ASP:HB3	1:F:534:GLU:OE1	2.18	0.44
1:B:374:GLY:C	1:B:376:LEU:N	2.75	0.44
1:B:375:ILE:HA	1:B:378:LEU:HG	1.99	0.44
1:C:524:GLU:CA	1:C:525:PRO:C	2.89	0.44
1:D:539:GLU:OE1	1:D:539:GLU:N	2.44	0.44
1:D:463:LEU:O	1:D:463:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:PHE:HA	1:B:468:ILE:O	2.17	0.43
1:A:421:PHE:HA	1:A:468:ILE:O	2.18	0.43
1:A:430:TYR:O	1:A:529:ARG:HD2	2.17	0.43
1:C:459:ALA:HA	1:C:460:PRO:HD3	1.88	0.43
1:E:435:GLY:HA2	1:E:525:PRO:HD2	2.00	0.43
1:F:446:GLU:HB3	1:F:486:PHE:CE2	2.53	0.43
1:F:519:HIS:N	1:F:520:PRO:HD3	2.33	0.43
1:B:497:TYR:CB	1:B:498:PRO:HD3	2.46	0.43
1:E:393:GLY:HA3	1:E:400:TYR:CE1	2.54	0.43
1:E:447:ARG:HG3	1:E:447:ARG:NH1	2.33	0.43
1:F:419:ASP:HB2	1:F:465:LYS:HB2	1.99	0.43
1:C:478:GLU:C	1:C:481:PRO:HD2	2.43	0.43
1:E:430:TYR:O	1:E:529:ARG:HD2	2.19	0.43
1:F:438:LYS:O	1:F:439:THR:OG1	2.33	0.42
1:F:482:ARG:HG3	1:F:482:ARG:NH1	2.32	0.42
1:B:422:VAL:HB	1:B:469:LEU:CD2	2.49	0.42
1:A:445:LEU:HB2	1:A:448:ASP:OD2	2.19	0.42
1:D:438:LYS:O	1:D:439:THR:OG1	2.34	0.42
1:F:532:ASN:O	1:F:533:HIS:C	2.63	0.42
1:C:393:GLY:HA3	1:C:400:TYR:CE1	2.55	0.42
1:C:397:ASP:HB3	1:F:534:GLU:CD	2.45	0.42
1:C:443:LEU:HD13	1:C:449:ALA:HA	2.01	0.42
1:F:496:ASP:O	1:F:497:TYR:C	2.61	0.42
1:A:446:GLU:HB3	1:A:486:PHE:CE2	2.55	0.42
1:E:445:LEU:HB2	1:E:448:ASP:OD2	2.20	0.42
1:F:438:LYS:HG2	1:F:524:GLU:OE1	2.19	0.41
1:C:419:ASP:HB2	1:C:465:LYS:HB3	2.01	0.41
1:E:524:GLU:CA	1:E:525:PRO:C	2.92	0.41
1:B:482:ARG:HG2	1:B:482:ARG:NH1	2.35	0.41
1:B:524:GLU:CA	1:B:525:PRO:C	2.86	0.41
1:C:458:ILE:O	1:C:458:ILE:HG22	2.19	0.41
1:D:419:ASP:HB2	1:D:465:LYS:CB	2.48	0.41
1:B:438:LYS:O	1:B:439:THR:OG1	2.30	0.41
1:A:492:ARG:HD3	1:A:500:LEU:HD21	2.02	0.41
1:B:393:GLY:HA3	1:B:400:TYR:CE1	2.55	0.41
1:C:430:TYR:O	1:C:529:ARG:HD2	2.20	0.41
1:D:524:GLU:CA	1:D:525:PRO:C	2.89	0.41
1:A:436:HIS:HD2	1:A:437:ILE:O	2.04	0.40
1:C:436:HIS:HD2	1:C:437:ILE:O	2.04	0.40
1:A:377:GLU:O	1:A:385:ALA:HA	2.20	0.40
1:D:443:LEU:HD13	1:D:449:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:LEU:HD21	1:D:544:ARG:CZ	2.52	0.40
1:E:533:HIS:CE1	1:E:535:ALA:HB3	2.56	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)
1:B:382:TYR:OH	1:F:524:GLU:OE1[5_554]	2.09	0.11

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	170/203 (84%)	158 (93%)	11 (6%)	1 (1%)	21	30
1	B	170/203 (84%)	156 (92%)	13 (8%)	1 (1%)	21	30
1	C	170/203 (84%)	157 (92%)	13 (8%)	0	100	100
1	D	170/203 (84%)	159 (94%)	11 (6%)	0	100	100
1	E	170/203 (84%)	160 (94%)	10 (6%)	0	100	100
1	F	170/203 (84%)	157 (92%)	12 (7%)	1 (1%)	21	30
All	All	1020/1218 (84%)	947 (93%)	70 (7%)	3 (0%)	36	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	TYR
1	B	497	TYR
1	F	463	LEU

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	155/179 (87%)	151 (97%)	4 (3%)	40	60
1	B	155/179 (87%)	152 (98%)	3 (2%)	50	69
1	C	155/179 (87%)	152 (98%)	3 (2%)	50	69
1	D	155/179 (87%)	151 (97%)	4 (3%)	40	60
1	E	155/179 (87%)	152 (98%)	3 (2%)	50	69
1	F	155/179 (87%)	153 (99%)	2 (1%)	61	78
All	All	930/1074 (87%)	911 (98%)	19 (2%)	48	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	A	463	LEU
1	A	482	ARG
1	A	540	LEU
1	B	377	GLU
1	B	416	ASN
1	B	543	PHE
1	C	416	ASN
1	C	540	LEU
1	C	543	PHE
1	D	377	GLU
1	D	416	ASN
1	D	463	LEU
1	D	543	PHE
1	E	416	ASN
1	E	476	SER
1	E	544	ARG
1	F	416	ASN
1	F	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	GLN
1	A	518	GLN
1	B	396	GLN
1	B	442	ASN
1	B	518	GLN
1	C	396	GLN
1	C	518	GLN
1	D	396	GLN
1	D	442	ASN
1	D	518	GLN
1	E	396	GLN
1	E	442	ASN
1	E	518	GLN
1	F	396	GLN
1	F	518	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](#)

6 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	E	1545	-	4,4,4	1.47	0	6,6,6	0.47	0
2	PO4	A	1545	-	4,4,4	1.52	0	6,6,6	0.44	0
2	PO4	F	1545	-	4,4,4	1.46	0	6,6,6	0.48	0
2	PO4	D	1545	-	4,4,4	1.45	1 (25%)	6,6,6	0.44	0
2	PO4	B	1545	-	4,4,4	1.48	0	6,6,6	0.44	0
2	PO4	C	1545	-	4,4,4	1.66	1 (25%)	6,6,6	0.46	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1545	PO4	P-O4	-2.26	1.48	1.54
2	D	1545	PO4	P-O4	-2.00	1.48	1.54

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	172/203 (84%)	1.03	29 (16%) 4 4	31, 52, 89, 104	0
1	B	172/203 (84%)	0.88	29 (16%) 4 4	32, 54, 91, 103	0
1	C	172/203 (84%)	0.71	24 (13%) 6 5	33, 49, 93, 110	0
1	D	172/203 (84%)	0.55	18 (10%) 11 10	31, 47, 92, 100	0
1	E	172/203 (84%)	0.70	18 (10%) 11 10	36, 53, 90, 101	0
1	F	172/203 (84%)	0.78	16 (9%) 14 13	36, 52, 88, 107	0
All	All	1032/1218 (84%)	0.78	134 (12%) 7 6	31, 51, 91, 110	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	463	LEU	8.3
1	C	463	LEU	7.4
1	A	463	LEU	6.2
1	C	460	PRO	6.2
1	B	545	LEU	5.9
1	C	461	CYS	5.9
1	A	374	GLY	5.6
1	D	463	LEU	5.5
1	E	463	LEU	5.4
1	B	374	GLY	5.4
1	A	545	LEU	5.1
1	B	463	LEU	4.9
1	C	462	SER	4.9
1	A	464	ASP	4.7
1	A	462	SER	4.6
1	D	542	THR	4.5
1	C	458	ILE	4.5
1	D	545	LEU	4.4
1	C	465	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	459	ALA	4.3
1	D	460	PRO	4.3
1	D	461	CYS	4.3
1	D	458	ILE	4.2
1	B	461	CYS	4.1
1	E	461	CYS	4.1
1	B	462	SER	4.1
1	E	464	ASP	4.0
1	C	459	ALA	3.9
1	B	498	PRO	3.9
1	A	459	ALA	3.8
1	B	464	ASP	3.8
1	E	374	GLY	3.8
1	B	543	PHE	3.6
1	A	540	LEU	3.6
1	C	374	GLY	3.5
1	F	545	LEU	3.5
1	A	458	ILE	3.5
1	F	460	PRO	3.4
1	D	374	GLY	3.4
1	B	496	ASP	3.4
1	E	493	ALA	3.2
1	C	464	ASP	3.2
1	D	417	ILE	3.2
1	E	459	ALA	3.2
1	F	461	CYS	3.2
1	D	543	PHE	3.2
1	B	495	ASN	3.1
1	A	460	PRO	3.1
1	D	462	SER	3.1
1	B	376	LEU	3.1
1	C	493	ALA	3.1
1	A	499	SER	3.0
1	A	496	ASP	3.0
1	B	378	LEU	3.0
1	F	467	VAL	3.0
1	B	476	SER	3.0
1	E	460	PRO	2.9
1	F	459	ALA	2.9
1	B	458	ILE	2.9
1	B	497	TYR	2.9
1	C	456	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	545	LEU	2.9
1	B	375	ILE	2.9
1	F	374	GLY	2.8
1	A	461	CYS	2.8
1	C	543	PHE	2.8
1	A	495	ASN	2.8
1	F	420	LYS	2.8
1	F	458	ILE	2.8
1	A	378	LEU	2.8
1	E	477	SER	2.7
1	A	476	SER	2.7
1	A	467	VAL	2.6
1	A	498	PRO	2.6
1	A	491	ASP	2.6
1	B	460	PRO	2.5
1	A	497	TYR	2.5
1	B	380	GLY	2.5
1	F	524	GLU	2.5
1	E	376	LEU	2.5
1	A	543	PHE	2.5
1	C	467	VAL	2.5
1	A	500	LEU	2.5
1	B	385	ALA	2.5
1	A	494	VAL	2.4
1	C	454	LEU	2.4
1	F	376	LEU	2.4
1	E	482	ARG	2.4
1	F	466	ARG	2.4
1	B	416	ASN	2.4
1	D	540	LEU	2.4
1	F	500	LEU	2.4
1	C	447	ARG	2.4
1	A	465	LYS	2.3
1	B	540	LEU	2.3
1	A	501	TYR	2.3
1	B	542	THR	2.3
1	C	417	ILE	2.3
1	B	518	GLN	2.3
1	F	543	PHE	2.3
1	B	491	ASP	2.3
1	F	465	LYS	2.3
1	B	459	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	535	ALA	2.3
1	A	454	LEU	2.3
1	C	457	PRO	2.3
1	E	543	PHE	2.2
1	E	532	ASN	2.2
1	C	415	SER	2.2
1	D	420	LYS	2.2
1	D	482	ARG	2.2
1	C	542	THR	2.2
1	B	544	ARG	2.2
1	B	465	LYS	2.2
1	E	462	SER	2.2
1	E	542	THR	2.2
1	B	457	PRO	2.2
1	D	541	LYS	2.2
1	C	420	LYS	2.1
1	D	455	LYS	2.1
1	F	542	THR	2.1
1	A	544	ARG	2.1
1	C	376	LEU	2.1
1	C	455	LYS	2.1
1	E	458	ILE	2.1
1	A	416	ASN	2.1
1	D	419	ASP	2.1
1	D	416	ASN	2.1
1	A	379	ILE	2.0
1	E	417	ILE	2.0
1	B	382	TYR	2.0
1	A	420	LYS	2.0
1	E	540	LEU	2.0
1	E	457	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	D	1545	5/5	0.92	0.18	51,53,55,56	0
2	PO4	E	1545	5/5	0.92	0.12	71,71,73,73	0
2	PO4	A	1545	5/5	0.93	0.16	48,48,52,54	0
2	PO4	B	1545	5/5	0.93	0.11	53,54,57,57	0
2	PO4	F	1545	5/5	0.96	0.10	49,49,53,53	0
2	PO4	C	1545	5/5	0.97	0.10	48,48,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.