



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:19 PM UTC

PDB ID : 2IKQ / pdb_00002ikq
Title : Crystal structure of mouse Sts-1 PGM domain in complex with phosphate
Authors : Chen, Y.; Nassar, N.
Deposited on : 2006-10-02
Resolution : 2.61 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

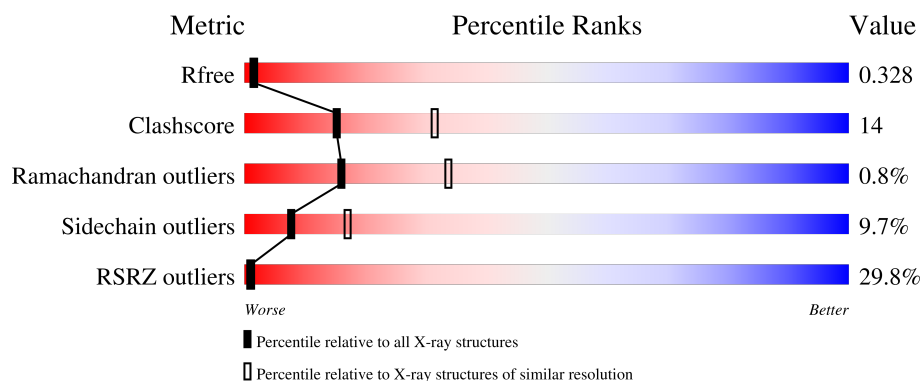
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	270	38% 66% 25% 6% .
1	B	270	28% 67% 23% 5% 5%
1	M	270	20% 69% 23% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6128 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 Suppressor of T-cell receptor signaling 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2065	1312	362	376	15			
1	B	256	Total	C	N	O	S	0	0	0
			2012	1277	351	369	15			
1	M	258	Total	C	N	O	S	0	0	0
			2026	1286	353	372	15			

- 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	B	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		

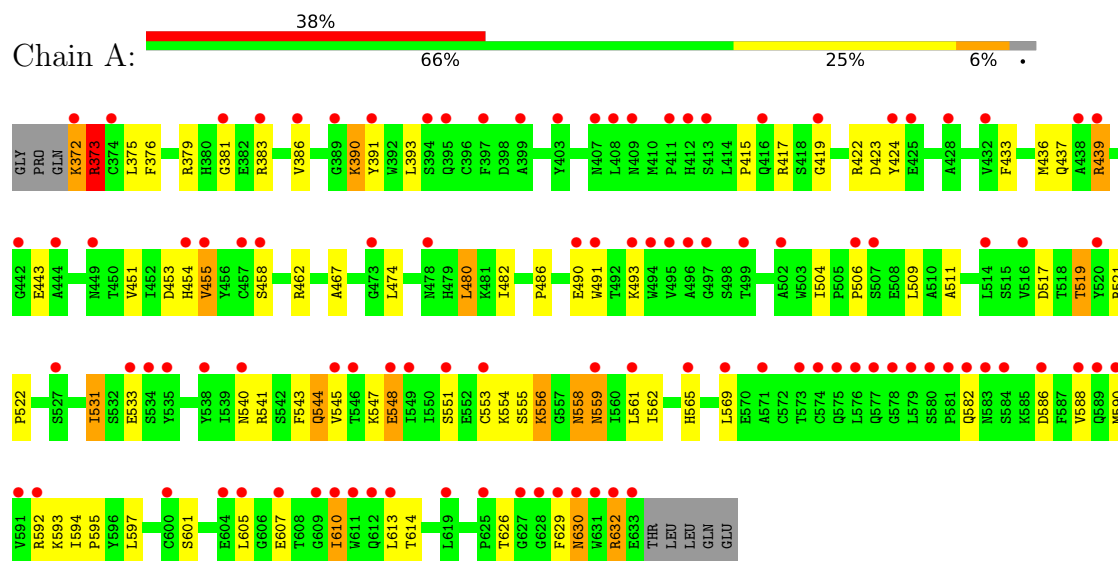
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	3	Total 3	O 3	0	0
3	M	3	Total 3	O 3	0	0

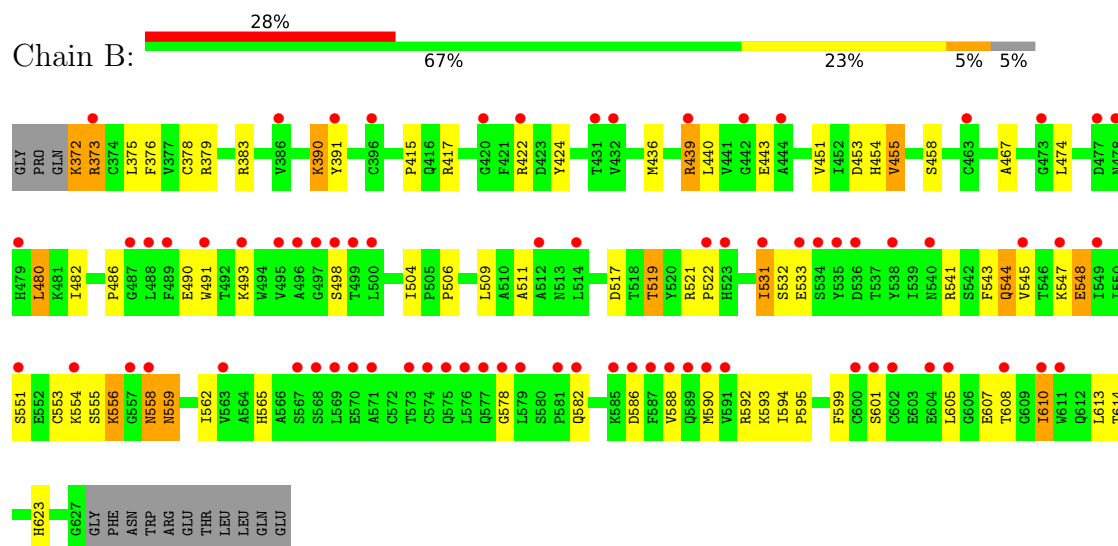
3 Residue-property plots

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: Suppressor of T-cell receptor signaling 1

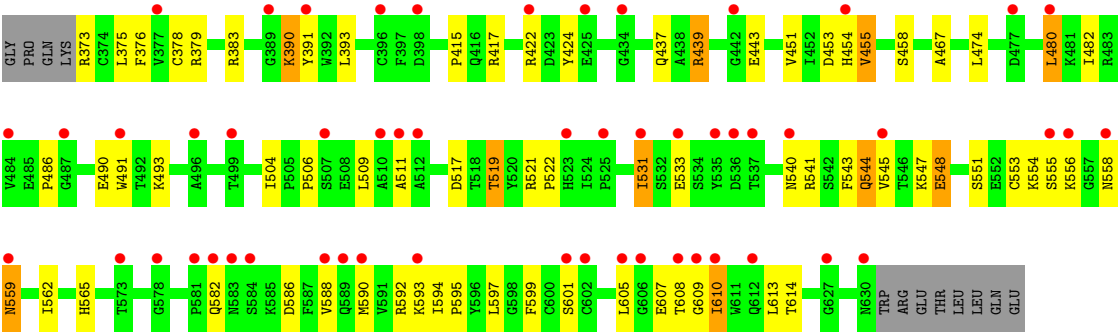


• Molecule 1: Suppressor of T-cell receptor signaling 1



• Molecule 1: Suppressor of T-cell receptor signaling 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 74.67Å 101.28Å 90.00° 100.79° 90.00°	Depositor
Resolution (Å)	99.50 – 2.61 99.49 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.6 (99.50-2.61) 97.5 (99.49-2.61)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	0.63	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.248 , 0.275 0.310 , 0.328	Depositor DCC
R_{free} test set	1293 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	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	0.89	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: 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	0.81	1/2118 (0.0%)	1.04	7/2877 (0.2%)
1	B	0.64	0/2062	0.99	4/2801 (0.1%)
1	M	0.57	0/2077	0.97	4/2822 (0.1%)
All	All	0.68	1/6257 (0.0%)	1.00	15/8500 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	ARG	CA-C	7.18	1.61	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ARG	N-CA-CB	-6.80	99.89	110.57
1	A	559	ASN	N-CA-C	6.25	119.42	110.10
1	B	559	ASN	N-CA-C	6.01	118.97	109.96
1	M	383	ARG	N-CA-CB	-5.83	101.41	110.57
1	M	559	ASN	N-CA-C	5.81	118.76	110.10
1	A	373	ARG	CG-CD-NE	-5.75	99.35	112.00
1	M	521	ARG	CA-C-N	5.72	125.67	119.78
1	M	521	ARG	C-N-CA	5.72	125.67	119.78
1	A	521	ARG	CA-C-N	5.59	125.54	119.78
1	A	521	ARG	C-N-CA	5.59	125.54	119.78
1	B	383	ARG	N-CA-CB	-5.56	101.85	110.57
1	B	521	ARG	CA-C-N	5.43	125.37	119.78
1	B	521	ARG	C-N-CA	5.43	125.37	119.78
1	A	632	ARG	N-CA-C	5.29	116.70	109.18
1	A	386	VAL	N-CA-C	-5.10	107.42	111.81

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	2065	0	2043	76	1
1	B	2012	0	2000	65	4
1	M	2026	0	2005	40	4
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	M	5	0	0	0	0
3	A	4	0	0	1	0
3	B	3	0	0	0	0
3	M	3	0	0	0	0
All	All	6128	0	6048	165	5

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 14.

All (165) 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:372:LYS:O	1:A:373:ARG:HG3	1.53	1.09
1:B:372:LYS:O	1:B:373:ARG:HG3	1.55	1.06
1:M:531:ILE:H	1:M:531:ILE:HD12	1.39	0.88
1:A:531:ILE:H	1:A:531:ILE:HD12	1.39	0.88
1:B:372:LYS:O	1:B:372:LYS:HG2	1.74	0.87
1:A:372:LYS:O	1:A:372:LYS:HG2	1.72	0.87
1:B:531:ILE:HD12	1:B:531:ILE:H	1.39	0.85
1:M:541:ARG:O	1:M:545:VAL:HG23	1.78	0.82
1:A:629:PHE:CE2	1:B:593:LYS:HE2	2.16	0.80
1:A:541:ARG:O	1:A:545:VAL:HG23	1.80	0.80
1:B:541:ARG:O	1:B:545:VAL:HG23	1.81	0.80
1:A:629:PHE:CE1	1:B:593:LYS:HG3	2.18	0.79
1:B:453:ASP:O	1:B:454:HIS:HD2	1.66	0.78
1:A:632:ARG:NH2	1:B:595:PRO:HD3	1.99	0.78
1:M:453:ASP:O	1:M:454:HIS:HD2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASP:O	1:A:454:HIS:HD2	1.67	0.77
1:B:372:LYS:C	1:B:373:ARG:HG3	2.13	0.73
1:B:373:ARG:HG2	1:B:373:ARG:HH11	1.54	0.73
1:A:372:LYS:C	1:A:373:ARG:HG3	2.11	0.72
1:A:373:ARG:HH11	1:A:373:ARG:HG2	1.56	0.70
1:A:415:PRO:HD2	1:A:424:TYR:OH	1.93	0.68
1:A:588:VAL:HG12	1:A:592:ARG:NH2	2.09	0.68
1:A:629:PHE:CZ	1:B:593:LYS:HE2	2.28	0.67
1:B:453:ASP:C	1:B:454:HIS:HD2	2.03	0.66
1:A:453:ASP:C	1:A:454:HIS:HD2	2.02	0.65
1:B:415:PRO:HD2	1:B:424:TYR:OH	1.97	0.65
1:M:415:PRO:HD2	1:M:424:TYR:OH	1.97	0.65
1:A:629:PHE:CZ	1:B:593:LYS:HG3	2.32	0.65
1:A:390:LYS:HD3	1:A:391:TYR:CZ	2.31	0.65
1:M:588:VAL:HG12	1:M:592:ARG:NH2	2.13	0.64
1:B:390:LYS:HD3	1:B:391:TYR:CZ	2.33	0.64
1:A:373:ARG:HG2	1:A:373:ARG:NH1	2.12	0.64
1:M:390:LYS:HD3	1:M:391:TYR:CZ	2.33	0.64
1:M:453:ASP:C	1:M:454:HIS:HD2	2.05	0.64
1:M:517:ASP:OD1	1:M:519:THR:HB	1.98	0.63
1:A:372:LYS:HG2	1:A:558:ASN:ND2	2.13	0.63
1:B:588:VAL:HG12	1:B:592:ARG:NH2	2.14	0.63
1:A:517:ASP:OD1	1:A:519:THR:HB	1.99	0.63
1:A:453:ASP:C	1:A:454:HIS:CD2	2.77	0.62
1:B:517:ASP:OD1	1:B:519:THR:HB	1.99	0.62
1:A:632:ARG:HH22	1:B:595:PRO:HD3	1.65	0.62
1:B:373:ARG:HG2	1:B:373:ARG:NH1	2.13	0.62
1:B:372:LYS:HG2	1:B:558:ASN:ND2	2.15	0.61
1:B:453:ASP:C	1:B:454:HIS:CD2	2.78	0.61
1:M:455:VAL:HG12	1:M:480:LEU:HD22	1.82	0.61
1:M:453:ASP:C	1:M:454:HIS:CD2	2.79	0.60
1:A:630:ASN:C	1:A:630:ASN:ND2	2.59	0.59
1:B:455:VAL:HG12	1:B:480:LEU:HD22	1.84	0.59
1:A:373:ARG:CZ	1:A:373:ARG:CB	2.77	0.59
1:A:455:VAL:HG12	1:A:480:LEU:HD22	1.83	0.59
1:M:376:PHE:HD1	1:M:601:SER:HB3	1.67	0.59
1:A:376:PHE:HD1	1:A:601:SER:HB3	1.66	0.58
1:B:376:PHE:HD1	1:B:601:SER:HB3	1.67	0.58
1:A:582:GLN:NE2	1:A:590:MET:SD	2.77	0.58
1:A:629:PHE:CE1	1:B:593:LYS:CG	2.86	0.58
1:A:373:ARG:NH1	1:A:373:ARG:CG	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:GLN:NE2	1:B:590:MET:SD	2.76	0.56
1:B:453:ASP:O	1:B:454:HIS:CD2	2.55	0.56
1:A:372:LYS:O	1:A:372:LYS:CG	2.50	0.56
1:B:373:ARG:NH1	1:B:373:ARG:CG	2.68	0.55
1:A:453:ASP:O	1:A:454:HIS:CD2	2.56	0.55
1:A:551:SER:HA	1:A:554:LYS:HE3	1.89	0.54
1:A:630:ASN:C	1:A:630:ASN:HD22	2.16	0.53
1:B:373:ARG:CB	1:B:373:ARG:CZ	2.83	0.53
1:M:453:ASP:O	1:M:454:HIS:CD2	2.56	0.53
1:M:551:SER:HA	1:M:554:LYS:HE3	1.88	0.53
1:B:551:SER:HA	1:B:554:LYS:HE3	1.89	0.52
1:A:506:PRO:O	1:A:509:LEU:HB2	2.09	0.52
1:B:439:ARG:O	1:B:443:GLU:HG3	2.10	0.52
1:M:506:PRO:O	1:M:509:LEU:HB2	2.09	0.52
1:B:531:ILE:H	1:B:531:ILE:CD1	2.16	0.52
1:M:582:GLN:NE2	1:M:590:MET:SD	2.81	0.51
1:A:439:ARG:O	1:A:443:GLU:HG3	2.11	0.51
1:M:506:PRO:HA	1:M:509:LEU:HD12	1.93	0.51
1:B:372:LYS:O	1:B:372:LYS:CG	2.51	0.50
1:B:506:PRO:O	1:B:509:LEU:HB2	2.12	0.50
1:A:531:ILE:H	1:A:531:ILE:CD1	2.15	0.49
1:B:454:HIS:ND1	1:B:553:CYS:SG	2.77	0.49
1:A:390:LYS:HD3	1:A:391:TYR:CE2	2.47	0.49
1:M:439:ARG:O	1:M:443:GLU:HG3	2.12	0.49
1:A:467:ALA:HB3	1:A:482:ILE:HD13	1.93	0.49
1:B:504:ILE:HG22	1:B:509:LEU:HG	1.94	0.49
1:B:590:MET:O	1:B:593:LYS:HB2	2.12	0.49
1:A:504:ILE:HG22	1:A:509:LEU:HG	1.94	0.49
1:A:506:PRO:HA	1:A:509:LEU:HD12	1.94	0.49
1:A:590:MET:O	1:A:593:LYS:HB2	2.13	0.49
1:A:417:ARG:HG2	1:A:504:ILE:HD11	1.94	0.48
1:M:454:HIS:ND1	1:M:553:CYS:SG	2.78	0.48
1:M:504:ILE:HG22	1:M:509:LEU:HG	1.95	0.48
1:A:462:ARG:NH2	2:A:101:PO4:O2	2.40	0.48
1:M:375:LEU:HD11	1:M:562:ILE:HD12	1.96	0.48
1:B:506:PRO:HA	1:B:509:LEU:HD12	1.95	0.48
1:B:417:ARG:HG2	1:B:504:ILE:HD11	1.96	0.48
1:A:375:LEU:HD11	1:A:562:ILE:HD12	1.96	0.48
1:B:467:ALA:HB3	1:B:482:ILE:HD13	1.96	0.48
1:A:491:TRP:CZ2	1:A:493:LYS:HD2	2.49	0.48
1:M:390:LYS:HD3	1:M:391:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ILE:HG22	3:A:4:HOH:O	2.14	0.47
1:B:390:LYS:HD3	1:B:391:TYR:CE2	2.49	0.47
1:A:467:ALA:CB	1:A:482:ILE:HD13	2.44	0.47
1:B:590:MET:HG3	1:B:593:LYS:HD2	1.95	0.47
1:M:544:GLN:O	1:M:548:GLU:HG2	2.15	0.47
1:M:417:ARG:HG2	1:M:504:ILE:HD11	1.95	0.47
1:M:491:TRP:CZ2	1:M:493:LYS:HD2	2.49	0.47
1:B:491:TRP:CZ2	1:B:493:LYS:HD2	2.50	0.47
1:M:467:ALA:HB3	1:M:482:ILE:HD13	1.96	0.47
1:A:629:PHE:CZ	1:B:593:LYS:CG	2.98	0.46
1:B:608:THR:OG1	1:B:610:ILE:HG13	2.15	0.46
1:A:590:MET:HG3	1:A:593:LYS:HD2	1.98	0.46
1:M:608:THR:OG1	1:M:610:ILE:HG13	2.15	0.46
1:A:626:THR:CG2	1:B:623:HIS:CD2	2.99	0.46
1:M:451:VAL:O	1:M:559:ASN:HB2	2.16	0.45
1:M:590:MET:O	1:M:593:LYS:HB2	2.17	0.45
1:B:375:LEU:HD11	1:B:562:ILE:HD12	1.98	0.45
1:B:467:ALA:CB	1:B:482:ILE:HD13	2.47	0.45
1:B:544:GLN:O	1:B:548:GLU:HG2	2.16	0.45
1:M:379:ARG:HD3	1:M:595:PRO:O	2.17	0.45
1:M:590:MET:HG3	1:M:593:LYS:HD2	1.99	0.45
1:A:379:ARG:HD3	1:A:595:PRO:O	2.17	0.44
1:A:544:GLN:O	1:A:548:GLU:HG2	2.16	0.44
1:A:632:ARG:HH22	1:B:595:PRO:CD	2.30	0.44
1:A:451:VAL:O	1:A:559:ASN:HB2	2.17	0.44
1:A:436:MET:HB2	1:B:436:MET:SD	2.57	0.44
1:A:630:ASN:ND2	1:A:630:ASN:O	2.43	0.44
1:A:454:HIS:ND1	1:A:553:CYS:SG	2.78	0.43
1:B:594:ILE:HA	1:B:595:PRO:HD3	1.78	0.43
1:B:376:PHE:CD1	1:B:601:SER:HB3	2.51	0.43
1:B:486:PRO:HD2	1:B:522:PRO:HB3	2.01	0.43
1:M:378:CYS:HB3	1:M:599:PHE:CD1	2.53	0.43
1:A:436:MET:HB2	1:B:436:MET:CE	2.49	0.43
1:M:467:ALA:CB	1:M:482:ILE:HD13	2.48	0.43
1:M:490:GLU:HB3	1:M:565:HIS:CG	2.54	0.42
1:A:376:PHE:CD1	1:A:601:SER:HB3	2.51	0.42
1:A:486:PRO:HD2	1:A:522:PRO:HB3	2.00	0.42
1:B:379:ARG:HD3	1:B:595:PRO:O	2.19	0.42
1:M:594:ILE:HA	1:M:595:PRO:HD3	1.79	0.42
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.87	0.42
1:M:486:PRO:HD2	1:M:522:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:SER:HA	1:B:554:LYS:CE	2.50	0.42
1:M:437:GLN:HB3	1:M:597:LEU:HD23	2.00	0.42
1:A:569:LEU:HD22	1:A:594:ILE:HD13	2.02	0.42
1:B:543:PHE:O	1:B:547:LYS:HB2	2.19	0.41
1:A:551:SER:HA	1:A:554:LYS:CE	2.50	0.41
1:B:451:VAL:O	1:B:559:ASN:HB2	2.19	0.41
1:A:490:GLU:HB3	1:A:565:HIS:CG	2.55	0.41
1:M:393:LEU:HD23	1:M:393:LEU:HA	1.86	0.41
1:A:381:GLY:HA2	1:A:597:LEU:CD2	2.51	0.41
1:B:490:GLU:HB3	1:B:565:HIS:CG	2.55	0.41
1:A:437:GLN:HB3	1:A:597:LEU:HD23	2.01	0.41
1:A:554:LYS:C	1:A:556:LYS:H	2.28	0.41
1:A:455:VAL:HA	1:A:561:LEU:O	2.21	0.41
1:A:543:PHE:O	1:A:547:LYS:HB2	2.20	0.41
1:A:433:PHE:HE1	1:B:440:LEU:HD12	1.86	0.41
1:A:381:GLY:HA2	1:A:597:LEU:HD22	2.01	0.41
1:A:419:GLY:HA3	1:A:423:ASP:OD2	2.21	0.41
1:A:629:PHE:CD1	1:B:593:LYS:HG2	2.55	0.41
1:B:378:CYS:HB3	1:B:599:PHE:CD1	2.55	0.41
1:M:543:PHE:O	1:M:547:LYS:HB2	2.21	0.41
1:A:433:PHE:HE1	1:B:440:LEU:CD1	2.34	0.41
1:M:551:SER:HA	1:M:554:LYS:CE	2.49	0.41
1:A:436:MET:SD	1:B:436:MET:HB2	2.60	0.40
1:A:594:ILE:HA	1:A:595:PRO:HD3	1.78	0.40
1:B:554:LYS:C	1:B:556:LYS:H	2.29	0.40
1:M:379:ARG:O	1:M:597:LEU:HA	2.21	0.40
1:A:379:ARG:O	1:A:597:LEU:HA	2.22	0.40

All (5) 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:578:GLY:O	1:M:391:TYR:OH[1_565]	1.90	0.30
1:A:540:ASN:ND2	1:A:629:PHE:CE1[4_545]	1.96	0.24
1:B:391:TYR:OH	1:M:540:ASN:ND2[3_555]	2.05	0.15
1:B:498:SER:OG	1:M:609:GLY:O[3_555]	2.15	0.05
1:B:532:SER:OG	1:M:554:LYS:NZ[3_555]	2.16	0.04

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	260/270 (96%)	246 (95%)	12 (5%)	2 (1%)	16	34
1	B	254/270 (94%)	240 (94%)	12 (5%)	2 (1%)	16	34
1	M	256/270 (95%)	241 (94%)	13 (5%)	2 (1%)	16	34
All	All	770/810 (95%)	727 (94%)	37 (5%)	6 (1%)	16	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	ALA
1	B	511	ALA
1	M	511	ALA
1	A	558	ASN
1	B	558	ASN
1	M	558	ASN

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	229/237 (97%)	206 (90%)	23 (10%)	7	16
1	B	225/237 (95%)	203 (90%)	22 (10%)	7	17
1	M	226/237 (95%)	205 (91%)	21 (9%)	8	18
All	All	680/711 (96%)	614 (90%)	66 (10%)	8	17

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LYS
1	A	373	ARG
1	A	390	LYS
1	A	422	ARG
1	A	439	ARG
1	A	455	VAL
1	A	458	SER
1	A	474	LEU
1	A	480	LEU
1	A	519	THR
1	A	531	ILE
1	A	533	GLU
1	A	544	GLN
1	A	548	GLU
1	A	555	SER
1	A	556	LYS
1	A	586	ASP
1	A	605	LEU
1	A	607	GLU
1	A	610	ILE
1	A	613	LEU
1	A	614	THR
1	A	630	ASN
1	B	372	LYS
1	B	373	ARG
1	B	390	LYS
1	B	422	ARG
1	B	439	ARG
1	B	455	VAL
1	B	458	SER
1	B	474	LEU
1	B	480	LEU
1	B	519	THR
1	B	531	ILE
1	B	533	GLU
1	B	544	GLN
1	B	548	GLU
1	B	555	SER
1	B	556	LYS
1	B	586	ASP
1	B	605	LEU
1	B	607	GLU

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Mol	Chain	Res	Type
1	B	610	ILE
1	B	613	LEU
1	B	614	THR
1	M	373	ARG
1	M	390	LYS
1	M	422	ARG
1	M	439	ARG
1	M	455	VAL
1	M	458	SER
1	M	474	LEU
1	M	480	LEU
1	M	519	THR
1	M	531	ILE
1	M	533	GLU
1	M	544	GLN
1	M	548	GLU
1	M	555	SER
1	M	556	LYS
1	M	586	ASP
1	M	605	LEU
1	M	607	GLU
1	M	610	ILE
1	M	613	LEU
1	M	614	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	577	GLN
1	B	577	GLN
1	M	577	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 [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	$\# Z > 2$
2	PO4	B	102	-	4,4,4	0.81	0	6,6,6	0.62	0
2	PO4	A	101	-	4,4,4	0.86	0	6,6,6	0.86	0
2	PO4	M	103	-	4,4,4	0.91	0	6,6,6	0.72	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	PO4	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	262/270 (97%)	1.88	102 (38%) 1 0	34, 68, 83, 89	3 (1%)
1	B	256/270 (94%)	1.57	75 (29%) 1 1	38, 68, 83, 89	2 (0%)
1	M	258/270 (95%)	1.29	54 (20%) 2 2	52, 68, 83, 89	3 (1%)
All	All	776/810 (95%)	1.58	231 (29%) 1 1	34, 68, 83, 89	8 (1%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	5.9
1	B	491	TRP	5.5
1	A	574	CYS	5.4
1	B	573	THR	5.0
1	A	627	GLY	4.8
1	B	574	CYS	4.5
1	A	610	ILE	4.5
1	A	583	ASN	4.5
1	A	588	VAL	4.4
1	M	610	ILE	4.4
1	M	582	GLN	4.4
1	A	538	TYR	4.3
1	B	534	SER	4.3
1	B	587	PHE	4.3
1	B	605	LEU	4.2
1	A	442	GLY	4.0
1	A	590	MET	4.0
1	B	578	GLY	4.0
1	B	538	TYR	3.9
1	A	553	CYS	3.9
1	M	608	THR	3.9
1	A	582	GLN	3.8
1	B	589	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	573	THR	3.8
1	B	590	MET	3.7
1	B	610	ILE	3.7
1	A	545	VAL	3.7
1	B	523	HIS	3.7
1	A	455	VAL	3.7
1	B	535	TYR	3.6
1	B	582	GLN	3.6
1	B	487	GLY	3.5
1	B	576	LEU	3.5
1	A	439	ARG	3.4
1	A	628	GLY	3.4
1	B	536	ASP	3.4
1	B	420	GLY	3.4
1	B	586	ASP	3.4
1	M	537	THR	3.3
1	A	576	LEU	3.2
1	M	584	SER	3.2
1	B	386	VAL	3.2
1	M	573	THR	3.2
1	M	589	GLN	3.2
1	M	627	GLY	3.2
1	M	510	ALA	3.2
1	M	540	ASN	3.2
1	A	454	HIS	3.2
1	A	473	GLY	3.2
1	A	499	THR	3.1
1	B	493	LYS	3.1
1	A	607	GLU	3.1
1	A	389	GLY	3.1
1	B	495	VAL	3.1
1	A	491	TRP	3.1
1	A	592	ARG	3.1
1	M	454	HIS	3.0
1	B	439	ARG	3.0
1	B	601	SER	3.0
1	M	442	GLY	3.0
1	A	559	ASN	3.0
1	A	625	PRO	3.0
1	A	428	ALA	3.0
1	A	408	LEU	2.9
1	B	585	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	557	GLY	2.9
1	B	500	LEU	2.9
1	A	581	PRO	2.9
1	B	498	SER	2.9
1	A	383	ARG	2.9
1	B	499	THR	2.9
1	A	551	SER	2.9
1	A	584	SER	2.9
1	M	630	ASN	2.9
1	B	391	TYR	2.9
1	B	496	ALA	2.9
1	A	609	GLY	2.9
1	A	569	LEU	2.9
1	B	591	VAL	2.9
1	M	491	TRP	2.8
1	B	477	ASP	2.8
1	A	372	LYS	2.8
1	A	444	ALA	2.8
1	A	496	ALA	2.8
1	A	493	LYS	2.8
1	M	605	LEU	2.8
1	B	463	CYS	2.8
1	A	577	GLN	2.8
1	A	589	GLN	2.8
1	M	525	PRO	2.8
1	A	540	ASN	2.7
1	A	395	GLN	2.7
1	B	602	CYS	2.7
1	B	444	ALA	2.7
1	A	457	CYS	2.7
1	A	600	CYS	2.7
1	A	449	ASN	2.7
1	A	611	TRP	2.7
1	M	583	ASN	2.7
1	A	549	ILE	2.6
1	A	535	TYR	2.6
1	A	412	HIS	2.6
1	M	609	GLY	2.6
1	B	611	TRP	2.6
1	M	581	PRO	2.6
1	A	409	ASN	2.6
1	A	432	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	522	PRO	2.6
1	B	568	SER	2.6
1	M	536	ASP	2.6
1	B	396	CYS	2.6
1	A	438	ALA	2.6
1	B	571	ALA	2.6
1	M	555	SER	2.5
1	A	419	GLY	2.5
1	B	581	PRO	2.5
1	B	588	VAL	2.5
1	A	527	SER	2.5
1	M	601	SER	2.5
1	A	631	TRP	2.5
1	B	569	LEU	2.5
1	M	377	VAL	2.5
1	A	571	ALA	2.5
1	M	507	SER	2.5
1	B	570	GLU	2.5
1	M	484	VAL	2.5
1	M	496	ALA	2.5
1	B	579	LEU	2.4
1	A	580	SER	2.4
1	B	604	GLU	2.4
1	A	591	VAL	2.4
1	M	511	ALA	2.4
1	A	561	LEU	2.4
1	M	612	GLN	2.4
1	A	495	VAL	2.4
1	A	516	VAL	2.4
1	M	588	VAL	2.4
1	A	502	ALA	2.4
1	B	512	ALA	2.4
1	M	556	LYS	2.4
1	M	434	GLY	2.4
1	M	545	VAL	2.4
1	M	531	ILE	2.3
1	A	546	THR	2.3
1	B	479	HIS	2.3
1	A	533	GLU	2.3
1	A	458	SER	2.3
1	B	551	SER	2.3
1	A	575	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	632	ARG	2.3
1	B	545	VAL	2.3
1	A	407	ASN	2.3
1	M	558	ASN	2.3
1	B	547	LYS	2.3
1	M	602	CYS	2.3
1	A	397	PHE	2.3
1	M	523	HIS	2.3
1	M	499	THR	2.3
1	A	478	ASN	2.3
1	A	579	LEU	2.3
1	B	558	ASN	2.3
1	A	534	SER	2.3
1	A	586	ASP	2.3
1	A	612	GLN	2.3
1	B	442	GLY	2.3
1	B	497	GLY	2.3
1	M	487	GLY	2.3
1	A	391	TYR	2.2
1	A	424	TYR	2.2
1	A	411	PRO	2.2
1	B	514	LEU	2.2
1	A	399	ALA	2.2
1	B	600	CYS	2.2
1	M	396	CYS	2.2
1	B	608	THR	2.2
1	M	391	TYR	2.2
1	B	478	ASN	2.2
1	B	473	GLY	2.2
1	M	389	GLY	2.2
1	M	477	ASP	2.2
1	M	606	GLY	2.2
1	A	494	TRP	2.2
1	A	633	GLU	2.2
1	B	431	THR	2.2
1	A	416	GLN	2.2
1	A	507	SER	2.2
1	M	480	LEU	2.2
1	A	386	VAL	2.2
1	B	549	ILE	2.2
1	A	413	SER	2.2
1	B	567	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	535	TYR	2.1
1	A	613	LEU	2.1
1	B	489	PHE	2.1
1	M	512	ALA	2.1
1	A	490	GLU	2.1
1	B	533	GLU	2.1
1	A	514	LEU	2.1
1	A	520	TYR	2.1
1	A	619	LEU	2.1
1	B	540	ASN	2.1
1	M	578	GLY	2.1
1	B	432	VAL	2.1
1	B	563	VAL	2.1
1	M	398	ASP	2.1
1	A	394	SER	2.1
1	A	425	GLU	2.1
1	M	425	GLU	2.1
1	M	593	LYS	2.1
1	B	575	GLN	2.1
1	B	577	GLN	2.1
1	M	590	MET	2.1
1	B	488	LEU	2.1
1	A	374	CYS	2.1
1	A	381	GLY	2.1
1	A	497	GLY	2.1
1	M	533	GLU	2.1
1	A	403	TYR	2.1
1	A	629	PHE	2.1
1	M	422	ARG	2.0
1	A	506	PRO	2.0
1	A	605	LEU	2.0
1	A	630	ASN	2.0
1	B	373	ARG	2.0
1	B	422	ARG	2.0
1	A	548	GLU	2.0
1	A	604	GLU	2.0
1	B	554	LYS	2.0
1	A	565	HIS	2.0
1	B	531	ILE	2.0
1	M	559	ASN	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	B	102	5/5	0.81	0.12	75,76,77,77	5
2	PO4	M	103	5/5	0.84	0.12	62,63,64,64	5
2	PO4	A	101	5/5	0.93	0.10	42,45,47,47	5

6.5 Other polymers [i](#)

There are no such residues in this entry.