



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:15 am GMT

PDB ID : 2IKQ
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

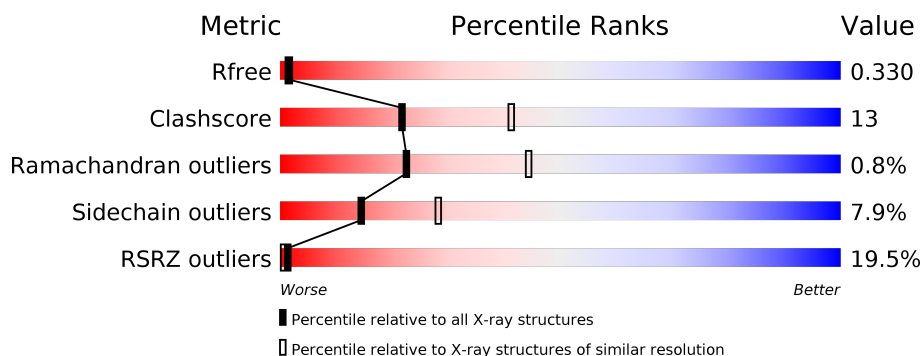
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>13%</div> <div>67%</div> <div>26%</div> <div>• •</div> </div>
1	B	270	<div> <div>23%</div> <div>69%</div> <div>23%</div> <div>• 5%</div> </div>
1	M	270	<div> <div>20%</div> <div>69%</div> <div>24%</div> <div>• •</div> </div>

2 Entry composition [i](#)

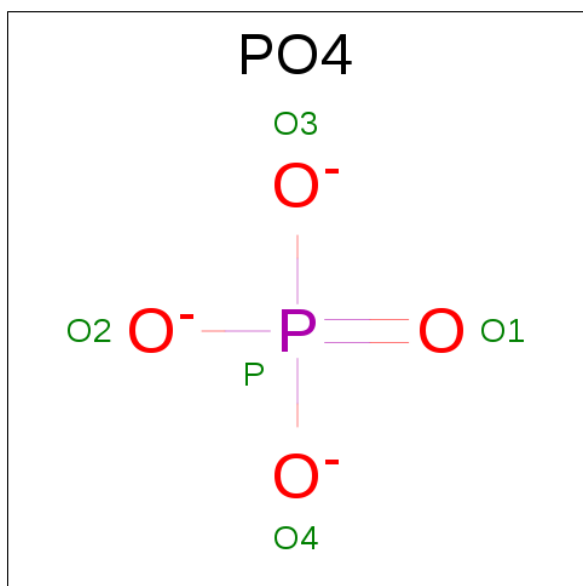
There are 3 unique types of molecules in this entry. The entry contains 6128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

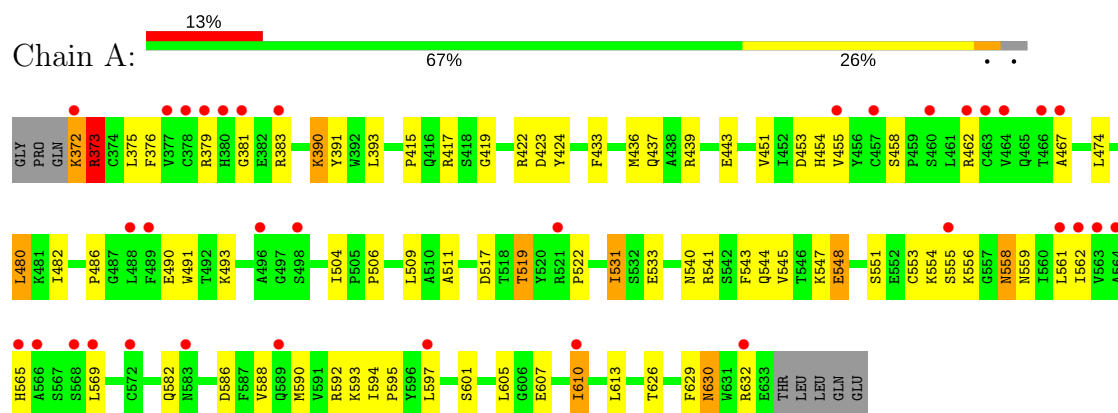
- Molecule 3 is water.

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

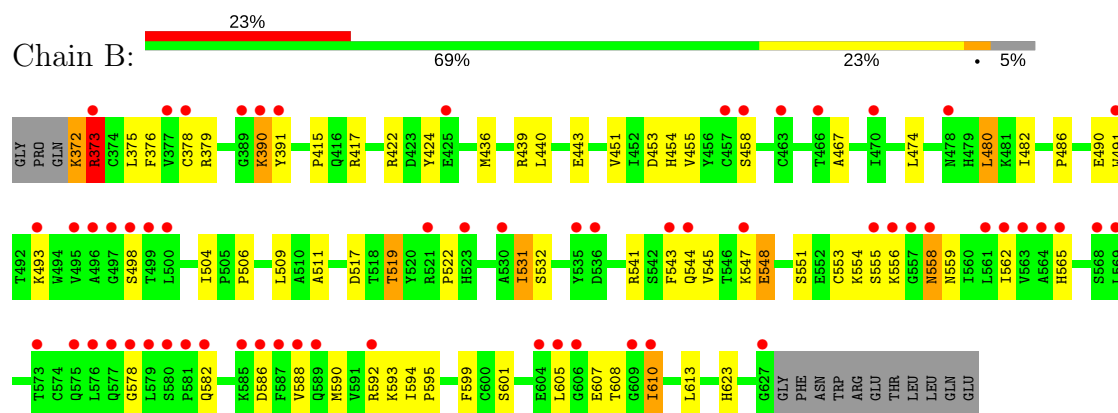
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

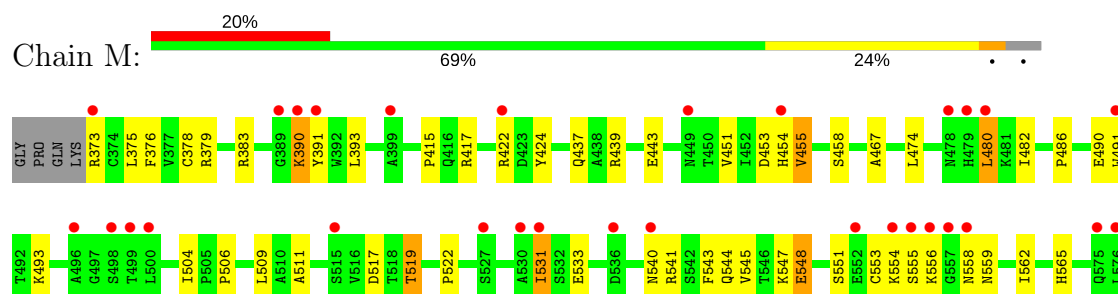
• Molecule 1: Suppressor of T-cell receptor signaling 1

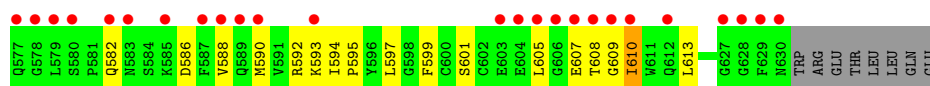


• Molecule 1: Suppressor of T-cell receptor signaling 1



• 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 30.77 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.6 (99.50-2.61) 97.6 (30.77-2.61)	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 0.306 , 0.330	Depositor DCC
R_{free} test set	1292 reflections (5.04%)	DCC
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 , 42.3	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 [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	0.65	0/2118	0.72	2/2877 (0.1%)
1	B	0.51	0/2062	0.67	1/2801 (0.0%)
1	M	0.46	0/2077	0.65	1/2822 (0.0%)
All	All	0.55	0/6257	0.68	4/8500 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ARG	N-CA-CB	-5.95	99.89	110.60
1	A	373	ARG	CG-CD-NE	-5.93	99.35	111.80
1	M	383	ARG	N-CA-CB	-5.11	101.41	110.60
1	B	373	ARG	CG-CD-NE	-5.02	101.26	111.80

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	2065	0	2043	75	1
1	B	2012	0	2000	64	4
1	M	2026	0	2005	40	4
2	A	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	163	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 13.

All (163) 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:HD12	1:A:531:ILE:H	1.39	0.88
1:B:372:LYS:HG2	1:B:372:LYS:O	1.74	0.87
1:A:372:LYS:HG2	1:A:372:LYS:O	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
1:A:453:ASP:O	1:A:454:HIS:HD2	1.67	0.77
1:B:373:ARG:HH11	1:B:373:ARG:HG2	1.54	0.73
1:A:373:ARG:HH11	1:A:373:ARG:HG2	1.56	0.70
1:B:372:LYS:C	1:B:373:ARG:HG3	2.13	0.69
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:372:LYS:C	1:A:373:ARG:HG3	2.11	0.67
1:A:629:PHE:CZ	1:B:593:LYS:HE2	2.28	0.67
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LYS:HD3	1:B:391:TYR:CZ	2.33	0.64
1:A:373:ARG:NH1	1:A:373:ARG:HG2	2.12	0.64
1:M:390:LYS:HD3	1:M:391:TYR:CZ	2.33	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: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:HD2	2.03	0.61
1:A:453:ASP:C	1:A:454:HIS:HD2	2.02	0.61
1:M:455:VAL:HG12	1:M:480:LEU:HD22	1.82	0.61
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:M:453:ASP:C	1:M:454:HIS:HD2	2.05	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:453:ASP:C	1:A:454:HIS:CD2	2.77	0.58
1:A:373:ARG:NH1	1:A:373:ARG:CG	2.66	0.57
1:B:453:ASP:C	1:B:454:HIS:CD2	2.78	0.56
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:M:453:ASP:C	1:M:454:HIS:CD2	2.79	0.55
1:B:373:ARG:CG	1:B:373:ARG:NH1	2.68	0.55
1:A:453:ASP:O	1:A:454:HIS:CD2	2.56	0.55
1:A:630:ASN:ND2	1:A:630:ASN:C	2.59	0.55
1:A:551:SER:HA	1:A:554:LYS:HE3	1.89	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ILE:CD1	1:B:531:ILE:H	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:CG	1:B:372:LYS:O	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:630:ASN:C	1:A:630:ASN:HD22	2.16	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:486:PRO:HD2	1:B:522:PRO:HB3	2.01	0.43
1:B:376:PHE:CD1	1:B:601:SER:HB3	2.51	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:486:PRO:HD2	1:A:522:PRO:HB3	2.00	0.42
1:A:376:PHE:CD1	1:A:601:SER:HB3	2.51	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:HA	1:A:393:LEU:HD23	1.87	0.42
1:M:486:PRO:HD2	1:M:522:PRO:HB3	2.00	0.42
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:HA	1:M:393:LEU:HD23	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:543:PHE:O	1:A:547:LYS:HB2	2.20	0.41
1:A:455:VAL:HA	1:A:561:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:HE1	1:B:440:LEU:HD12	1.86	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: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: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:594:ILE:HA	1:A:595:PRO:HD3	1.78	0.40
1:A:436:MET:SD	1:B:436:MET:HB2	2.60	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%)	22	44
1	B	254/270 (94%)	240 (94%)	12 (5%)	2 (1%)	22	44
1	M	256/270 (95%)	241 (94%)	13 (5%)	2 (1%)	22	44
All	All	770/810 (95%)	727 (94%)	37 (5%)	6 (1%)	22	44

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/237 (97%)	210 (92%)	19 (8%)	13	25
1	B	225/237 (95%)	208 (92%)	17 (8%)	15	30
1	M	226/237 (95%)	208 (92%)	18 (8%)	14	27
All	All	680/711 (96%)	626 (92%)	54 (8%)	14	28

All (54) 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	458	SER
1	A	474	LEU
1	A	480	LEU
1	A	519	THR
1	A	531	ILE
1	A	533	GLU
1	A	548	GLU
1	A	555	SER
1	A	556	LYS
1	A	586	ASP
1	A	605	LEU

Continued on next page...

Continued from previous page...

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	101	-	4,4,4	0.71	0	6,6,6	0.72	0
2	PO4	B	102	-	4,4,4	0.66	0	6,6,6	0.53	0
2	PO4	M	103	-	4,4,4	0.73	0	6,6,6	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	101	-	-	0/0/0/0	0/0/0/0
2	PO4	B	102	-	-	0/0/0/0	0/0/0/0
2	PO4	M	103	-	-	0/0/0/0	0/0/0/0

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%)	0.88	35 (13%) 4 2	49, 68, 83, 89	3 (1%)
1	B	256/270 (94%)	1.21	61 (23%) 1 0	52, 68, 83, 89	2 (0%)
1	M	258/270 (95%)	1.08	55 (21%) 1 0	52, 68, 83, 89	3 (1%)
All	All	776/810 (95%)	1.06	151 (19%) 1 0	49, 68, 83, 89	8 (1%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	582	GLN	8.1
1	M	630	ASN	6.4
1	B	557	GLY	6.2
1	B	498	SER	5.9
1	B	589	GLN	5.3
1	B	579	LEU	5.3
1	B	562	ILE	5.1
1	B	491	TRP	5.1
1	B	585	LYS	5.0
1	M	608	THR	4.9
1	M	593	LYS	4.8
1	M	555	SER	4.8
1	B	556	LYS	4.6
1	B	605	LEU	4.6
1	B	500	LEU	4.6
1	B	457	CYS	4.5
1	B	496	ALA	4.5
1	B	499	THR	4.5
1	M	558	ASN	4.4
1	B	555	SER	4.4
1	B	575	GLN	4.4
1	M	530	ALA	4.3
1	M	556	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	496	ALA	4.2
1	B	576	LEU	4.2
1	M	605	LEU	4.2
1	A	496	ALA	4.1
1	B	586	ASP	4.1
1	M	610	ILE	4.1
1	B	606	GLY	4.0
1	A	583	ASN	4.0
1	M	590	MET	3.9
1	B	582	GLN	3.9
1	B	610	ILE	3.7
1	M	609	GLY	3.7
1	M	373	ARG	3.7
1	M	499	THR	3.6
1	A	563	VAL	3.6
1	B	377	VAL	3.5
1	B	478	ASN	3.5
1	B	581	PRO	3.5
1	M	589	GLN	3.5
1	B	564	ALA	3.5
1	A	378	CYS	3.4
1	M	580	SER	3.4
1	M	579	LEU	3.4
1	B	378	CYS	3.4
1	M	627	GLY	3.4
1	B	493	LYS	3.3
1	M	612	GLN	3.3
1	B	604	GLU	3.3
1	M	500	LEU	3.2
1	M	390	LYS	3.2
1	B	535	TYR	3.2
1	A	564	ALA	3.2
1	A	381	GLY	3.2
1	M	557	GLY	3.2
1	A	377	VAL	3.2
1	B	530	ALA	3.2
1	A	568	SER	3.2
1	B	561	LEU	3.1
1	M	536	ASP	3.1
1	B	568	SER	3.1
1	M	527	SER	3.0
1	A	463	CYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	562	ILE	3.0
1	M	606	GLY	3.0
1	M	628	GLY	3.0
1	M	588	VAL	3.0
1	B	627	GLY	3.0
1	A	597	LEU	3.0
1	A	380	HIS	3.0
1	M	491	TRP	3.0
1	B	391	TYR	2.9
1	A	457	CYS	2.9
1	M	391	TYR	2.9
1	M	583	ASN	2.8
1	B	565	HIS	2.7
1	M	603	GLU	2.7
1	M	498	SER	2.7
1	A	379	ARG	2.7
1	B	497	GLY	2.7
1	B	558	ASN	2.7
1	M	552	GLU	2.7
1	B	569	LEU	2.7
1	A	466	THR	2.7
1	B	563	VAL	2.7
1	B	523	HIS	2.7
1	M	587	PHE	2.7
1	B	578	GLY	2.7
1	M	629	PHE	2.7
1	B	573	THR	2.6
1	M	449	ASN	2.6
1	M	577	GLN	2.6
1	B	587	PHE	2.6
1	A	498	SER	2.6
1	A	565	HIS	2.6
1	B	580	SER	2.6
1	M	454	HIS	2.6
1	M	479	HIS	2.6
1	B	495	VAL	2.5
1	B	466	THR	2.5
1	A	561	LEU	2.5
1	M	607	GLU	2.5
1	A	488	LEU	2.5
1	M	478	ASN	2.4
1	A	464	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	536	ASP	2.4
1	M	531	ILE	2.4
1	B	547	LYS	2.4
1	A	555	SER	2.4
1	B	544	GLN	2.4
1	B	577	GLN	2.4
1	B	389	GLY	2.4
1	M	578	GLY	2.4
1	A	572	CYS	2.4
1	M	389	GLY	2.3
1	A	566	ALA	2.3
1	M	515	SER	2.3
1	A	462	ARG	2.3
1	A	467	ALA	2.3
1	M	554	LYS	2.3
1	A	569	LEU	2.3
1	B	458	SER	2.3
1	M	399	ALA	2.3
1	B	470	ILE	2.3
1	B	373	ARG	2.3
1	B	521	ARG	2.3
1	B	592	ARG	2.3
1	M	480	LEU	2.3
1	M	540	ASN	2.3
1	A	372	LYS	2.3
1	B	390	LYS	2.2
1	A	383	ARG	2.2
1	M	575	GLN	2.2
1	B	588	VAL	2.2
1	B	609	GLY	2.2
1	A	455	VAL	2.2
1	M	422	ARG	2.2
1	A	632	ARG	2.2
1	A	489	PHE	2.1
1	B	463	CYS	2.1
1	A	521	ARG	2.1
1	A	610	ILE	2.1
1	A	460	SER	2.1
1	M	604	GLU	2.1
1	B	543	PHE	2.1
1	A	589	GLN	2.0
1	B	425	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	576	LEU	2.0
1	M	585	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	M	103	5/5	0.93	0.26	0.96	62,63,64,64	5
2	PO4	B	102	5/5	0.89	0.30	0.70	75,76,77,77	5
2	PO4	A	101	5/5	0.96	0.29	-0.99	42,45,47,47	5

6.5 Other polymers [i](#)

There are no such residues in this entry.