W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:05 AM GMT

PDB ID : 3DB1
Title : Crystal structure of the 2H-phosphatase domain of Sts-2 in complex with phosphate
Authors : Nassar, N.; Chen, Y.; Carpino, N.
Deposited on : 2008-05-30
Resolution : 2.77 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865
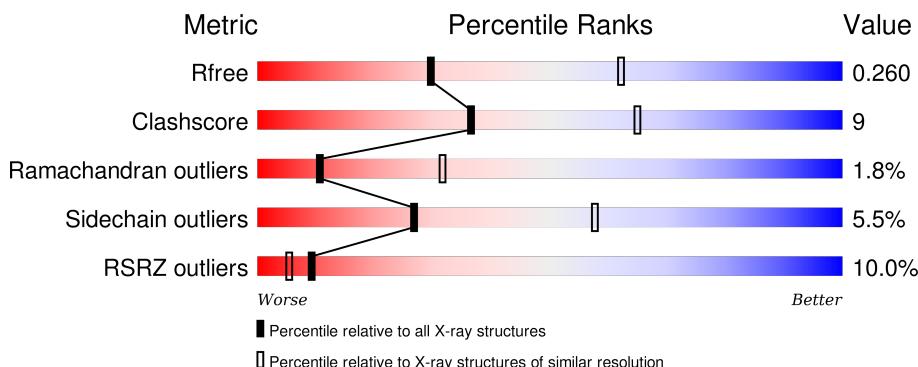
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
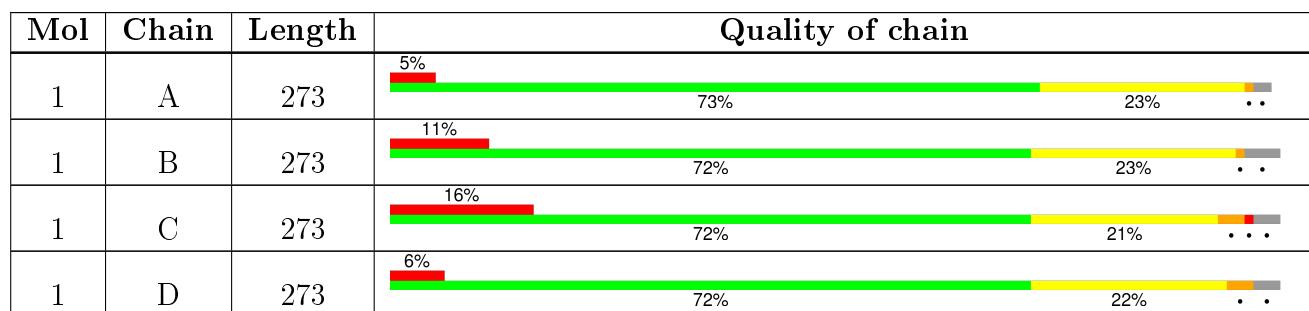
The reported resolution of this entry is 2.77 Å.

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		9
Ramachandran outliers		1.8%
Sidechain outliers		5.5%
RSRZ outliers		10.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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 <=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	273	5% 73% 23% ··
1	B	273	11% 72% 23% ··
1	C	273	16% 72% 21% ···
1	D	273	6% 72% 22% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8421 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.
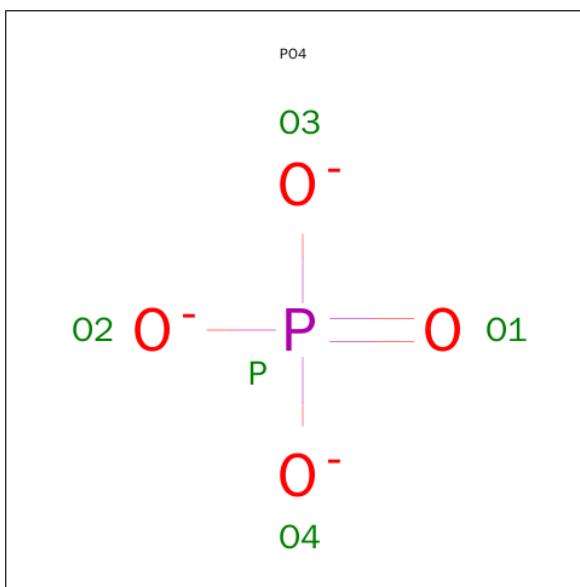
- Molecule 1 is a protein called STS-2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2115	1338	375	387	15			
1	B	263	Total	C	N	O	S	0	0	0
			2088	1321	371	381	15			
1	C	264	Total	C	N	O	S	0	0	0
			2096	1327	372	382	15			
1	D	265	Total	C	N	O	S	0	0	0
			2102	1330	373	384	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
A	351	MET	-	EXPRESSION TAG	UNP Q8BX41
A	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
A	353	SER	-	EXPRESSION TAG	UNP Q8BX41
A	364	ILE	VAL	CONFLICT	UNP Q8BX41
B	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
B	351	MET	-	EXPRESSION TAG	UNP Q8BX41
B	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
B	353	SER	-	EXPRESSION TAG	UNP Q8BX41
B	364	ILE	VAL	CONFLICT	UNP Q8BX41
C	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
C	351	MET	-	EXPRESSION TAG	UNP Q8BX41
C	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
C	353	SER	-	EXPRESSION TAG	UNP Q8BX41
C	364	ILE	VAL	CONFLICT	UNP Q8BX41
D	350	ALA	-	EXPRESSION TAG	UNP Q8BX41
D	351	MET	-	EXPRESSION TAG	UNP Q8BX41
D	352	GLY	-	EXPRESSION TAG	UNP Q8BX41
D	353	SER	-	EXPRESSION TAG	UNP Q8BX41
D	364	ILE	VAL	CONFLICT	UNP Q8BX41

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 4	O 3	P 1	0	0
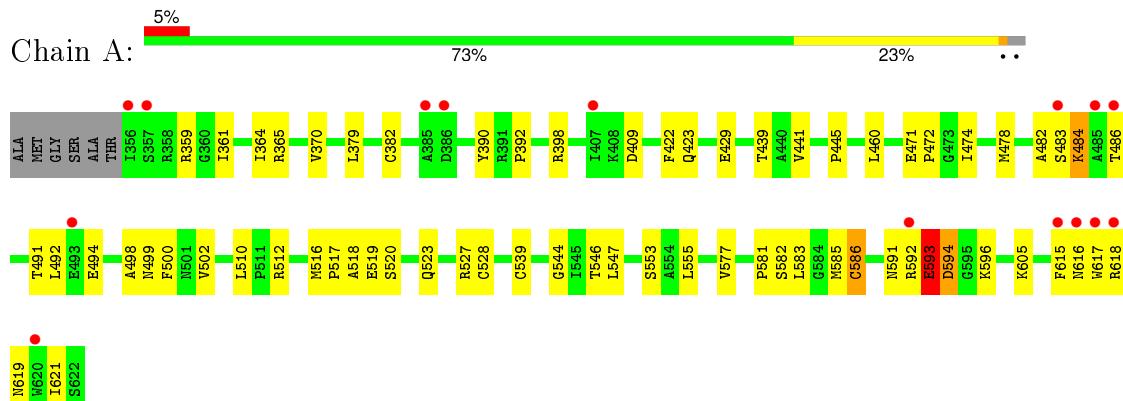
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	2	Total 2	O 2	0	0
3	C	2	Total 2	O 2	0	0
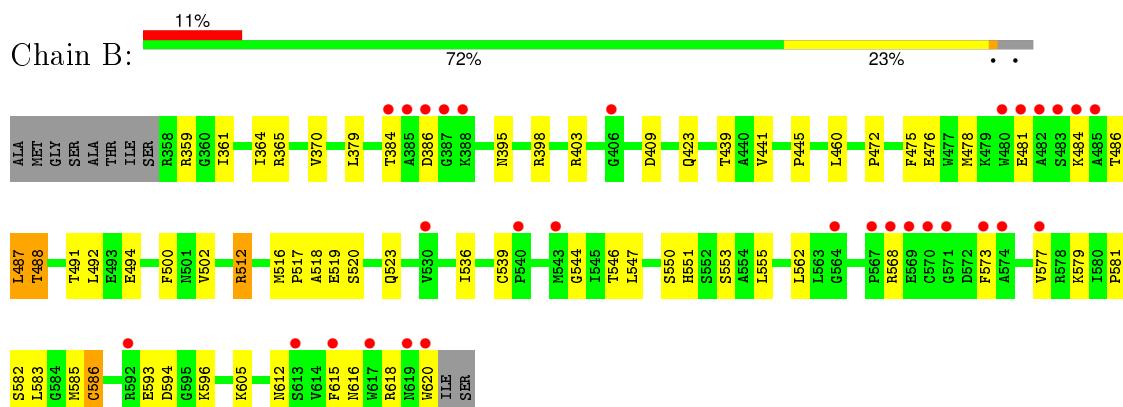
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
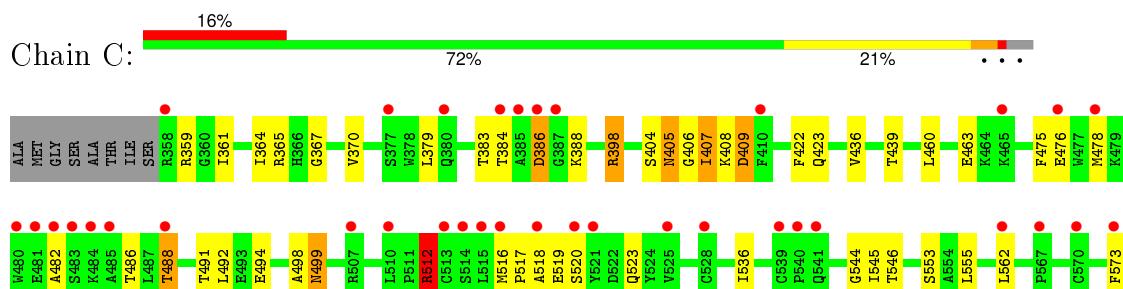
- Molecule 1: STS-2 protein

- Molecule 1: STS-2 protein

- Molecule 1: STS-2 protein

• Molecule 1: STS-2 protein

Chain D:
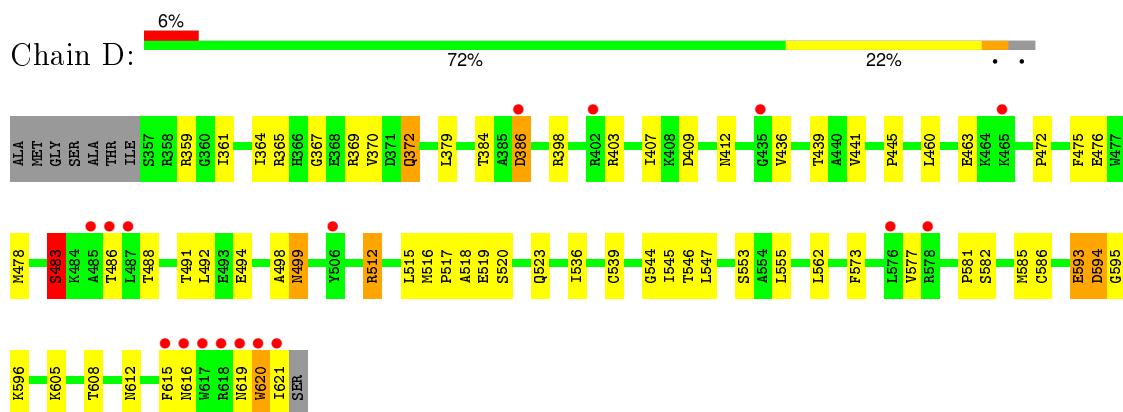
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.08Å 117.03Å 121.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.69 – 2.77 43.70 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.9 (43.69-2.77) 97.0 (43.70-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.270 0.235 , 0.260	Depositor DCC
R_{free} test set	1429 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	1 of 27988 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8421	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 32.15 % 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 9.8502e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.78	2/2163 (0.1%)	0.87	5/2929 (0.2%)
1	B	0.66	1/2136 (0.0%)	0.81	5/2894 (0.2%)
1	C	0.63	0/2144	0.69	4/2905 (0.1%)
1	D	0.67	1/2150 (0.0%)	0.74	5/2913 (0.2%)
All	All	0.69	4/8593 (0.0%)	0.78	19/11641 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	CYS	CB-SG	-7.40	1.69	1.82
1	B	586	CYS	CB-SG	-7.00	1.70	1.82
1	D	372	GLN	CG-CD	5.53	1.63	1.51
1	A	382	CYS	CB-SG	-5.07	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	ARG	NE-CZ-NH2	16.58	128.59	120.30
1	A	512	ARG	NE-CZ-NH1	-15.79	112.40	120.30
1	B	359	ARG	NE-CZ-NH2	15.65	128.12	120.30
1	B	359	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	A	512	ARG	CD-NE-CZ	8.47	135.46	123.60
1	D	512	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	512	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	512	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	359	ARG	CD-NE-CZ	7.11	133.56	123.60
1	A	359	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	359	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	359	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	512	ARG	NE-CZ-NH1	6.60	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	359	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	359	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	359	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	512	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	365	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2115	0	2114	47	0
1	B	2088	0	2086	43	0
1	C	2096	0	2097	41	0
1	D	2102	0	2102	51	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
All	All	8421	0	8399	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (159) 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:B:594:ASP:HB3	1:B:596:LYS:HG2	1.43	0.99
1:D:403:ARG:NH2	1:D:488:THR:O	2.01	0.93
1:A:616:ASN:HD21	1:A:619:ASN:CG	1.82	0.80
1:A:594:ASP:HB3	1:A:596:LYS:HG2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:TRP:O	1:A:621:ILE:HG23	1.84	0.78
1:A:618:ARG:O	1:A:621:ILE:HG12	1.87	0.74
1:C:478:MET:HB2	1:C:519:GLU:HG2	1.69	0.74
1:A:594:ASP:CB	1:A:596:LYS:HG2	2.18	0.73
1:D:619:ASN:O	1:D:620:TRP:HB2	1.90	0.72
1:B:615:PHE:HB2	1:D:581:PRO:HG3	1.73	0.71
1:D:594:ASP:CB	1:D:596:LYS:HG2	2.21	0.71
1:B:616:ASN:HD21	1:B:618:ARG:HB2	1.55	0.70
1:C:409:ASP:OD2	1:C:488:THR:HG21	1.91	0.69
1:A:478:MET:HB2	1:A:519:GLU:HG2	1.75	0.69
1:D:478:MET:HB2	1:D:519:GLU:HG2	1.75	0.69
1:B:478:MET:HB2	1:B:519:GLU:HG2	1.76	0.68
1:B:581:PRO:HG3	1:D:615:PHE:HB2	1.76	0.67
1:A:616:ASN:ND2	1:A:619:ASN:CG	2.48	0.66
1:D:594:ASP:HB3	1:D:596:LYS:HG2	1.76	0.66
1:B:484:LYS:HA	1:B:487:LEU:HD22	1.75	0.66
1:B:594:ASP:CB	1:B:596:LYS:HG2	2.23	0.66
1:A:615:PHE:CZ	1:A:617:TRP:HB2	2.30	0.66
1:C:492:LEU:H	1:C:492:LEU:HD12	1.62	0.65
1:A:592:ARG:NH1	1:A:592:ARG:HA	2.13	0.64
1:A:484:LYS:HD3	1:D:483:SER:H	1.63	0.63
1:B:579:LYS:NZ	1:D:620:TRP:CZ2	2.66	0.63
1:B:581:PRO:CG	1:D:615:PHE:HB2	2.29	0.63
1:C:404:SER:O	1:C:406:GLY:N	2.32	0.62
1:D:491:THR:OG1	1:D:494:GLU:HG3	1.99	0.62
1:D:619:ASN:O	1:D:620:TRP:CB	2.49	0.61
1:A:492:LEU:HD12	1:A:492:LEU:H	1.65	0.60
1:A:616:ASN:ND2	1:A:619:ASN:HB2	2.17	0.59
1:C:364:ILE:HG12	1:C:585:MET:HG2	1.85	0.59
1:B:612:ASN:HD21	1:D:582:SER:H	1.52	0.58
1:D:555:LEU:HD23	1:D:586:CYS:HB2	1.85	0.57
1:D:492:LEU:HD12	1:D:492:LEU:H	1.69	0.57
1:B:492:LEU:H	1:B:492:LEU:HD12	1.68	0.57
1:B:484:LYS:HA	1:B:487:LEU:CD2	2.34	0.57
1:A:592:ARG:HA	1:A:592:ARG:CZ	2.34	0.57
1:A:482:ALA:C	1:A:484:LYS:H	2.08	0.57
1:C:482:ALA:HB1	1:C:486:THR:OG1	2.04	0.56
1:B:361:ILE:HD13	1:B:546:THR:HB	1.87	0.56
1:C:491:THR:OG1	1:C:494:GLU:HG3	2.04	0.56
1:B:553:SER:HB2	1:B:573:PHE:HZ	1.70	0.55
1:C:553:SER:HB2	1:C:573:PHE:HZ	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:NH2	1:B:488:THR:O	2.40	0.54
1:C:423:GLN:HB3	1:C:583:LEU:HD23	1.89	0.54
1:D:520:SER:OG	1:D:523:GLN:HG3	2.08	0.54
1:D:364:ILE:HG12	1:D:585:MET:HG2	1.88	0.54
1:C:384:THR:OG1	1:C:386:ASP:HB3	2.07	0.54
1:C:594:ASP:HB2	1:C:596:LYS:HG2	1.89	0.54
1:A:491:THR:OG1	1:A:494:GLU:HG3	2.07	0.54
1:A:484:LYS:HD2	1:A:484:LYS:C	2.29	0.53
1:A:361:ILE:HD13	1:A:546:THR:HB	1.91	0.53
1:A:555:LEU:HD23	1:A:586:CYS:HB2	1.91	0.53
1:B:581:PRO:CD	1:D:615:PHE:HB2	2.39	0.52
1:A:364:ILE:HG12	1:A:585:MET:HG2	1.90	0.52
1:A:616:ASN:ND2	1:A:619:ASN:CB	2.72	0.52
1:A:618:ARG:NH1	1:C:602:PRO:HD3	2.25	0.52
1:B:384:THR:OG1	1:B:386:ASP:HB3	2.10	0.52
1:B:615:PHE:HB2	1:D:581:PRO:CG	2.39	0.52
1:B:520:SER:OG	1:B:523:GLN:HG3	2.10	0.52
1:A:615:PHE:HB2	1:C:581:PRO:HG3	1.92	0.52
1:D:616:ASN:HD21	1:D:619:ASN:HB2	1.75	0.52
1:C:404:SER:C	1:C:406:GLY:H	2.14	0.52
1:D:539:CYS:SG	1:D:539:CYS:O	2.67	0.52
1:D:594:ASP:HB2	1:D:596:LYS:HG2	1.92	0.51
1:B:395:ASN:HB2	1:D:608:THR:O	2.10	0.51
1:C:594:ASP:C	1:C:596:LYS:H	2.13	0.51
1:B:491:THR:OG1	1:B:494:GLU:HG3	2.10	0.51
1:A:593:GLU:O	1:A:594:ASP:C	2.50	0.51
1:B:364:ILE:HG12	1:B:585:MET:HG2	1.93	0.51
1:C:406:GLY:C	1:C:408:LYS:N	2.62	0.51
1:A:484:LYS:HB2	1:D:483:SER:HB3	1.92	0.50
1:A:553:SER:HA	1:A:577:VAL:HG11	1.93	0.50
1:A:472:PRO:HB2	1:A:510:LEU:O	2.11	0.50
1:D:593:GLU:O	1:D:595:GLY:N	2.44	0.50
1:C:618:ARG:C	1:C:620:TRP:H	2.15	0.49
1:D:361:ILE:HD13	1:D:546:THR:HB	1.94	0.49
1:C:555:LEU:HD23	1:C:586:CYS:HB2	1.94	0.49
1:B:555:LEU:HD23	1:B:586:CYS:HB2	1.94	0.49
1:B:439:THR:HG23	1:B:544:GLY:HA3	1.95	0.49
1:B:423:GLN:HB3	1:B:583:LEU:HD23	1.94	0.48
1:C:405:ASN:O	1:C:408:LYS:HG2	2.13	0.48
1:D:553:SER:HA	1:D:577:VAL:HG11	1.96	0.48
1:B:568:ARG:HH22	1:D:621:ILE:HG23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:ASP:CB	1:C:596:LYS:HG2	2.43	0.48
1:D:593:GLU:O	1:D:594:ASP:C	2.51	0.48
1:B:539:CYS:O	1:B:539:CYS:SG	2.72	0.48
1:C:361:ILE:HD13	1:C:546:THR:HB	1.96	0.47
1:A:582:SER:H	1:C:612:ASN:HD21	1.63	0.47
1:C:439:THR:HG23	1:C:544:GLY:HA3	1.96	0.47
1:B:579:LYS:NZ	1:D:620:TRP:CE2	2.76	0.47
1:B:616:ASN:ND2	1:B:618:ARG:HB2	2.28	0.47
1:A:423:GLN:HB3	1:A:583:LEU:HD23	1.97	0.47
1:D:369:ARG:HG3	1:D:372:GLN:HB2	1.96	0.47
1:D:436:VAL:HB	1:D:545:ILE:HD12	1.97	0.47
1:D:536:ILE:HD11	1:D:562:LEU:HD11	1.98	0.46
1:D:486:THR:HG21	1:D:515:LEU:HB2	1.97	0.46
1:C:367:GLY:HA2	1:C:582:SER:HB3	1.98	0.46
1:A:581:PRO:HG3	1:C:615:PHE:HB2	1.99	0.45
1:A:500:PHE:O	1:A:502:VAL:N	2.50	0.45
1:C:475:PHE:CG	1:C:476:GLU:N	2.85	0.45
1:C:383:THR:HA	1:C:388:LYS:O	2.16	0.45
1:C:404:SER:C	1:C:406:GLY:N	2.70	0.45
1:C:463:GLU:N	1:C:463:GLU:OE1	2.47	0.45
1:D:445:PRO:HD3	1:D:472:PRO:HA	1.98	0.44
1:B:475:PHE:CG	1:B:476:GLU:N	2.85	0.44
1:B:484:LYS:H	1:B:517:PRO:HB3	1.82	0.44
1:A:484:LYS:HB2	1:D:483:SER:CB	2.48	0.44
1:B:500:PHE:O	1:B:502:VAL:N	2.50	0.44
1:A:527:ARG:HG3	1:A:528:CYS:N	2.32	0.44
1:B:445:PRO:HD3	1:B:472:PRO:HA	1.99	0.44
1:D:463:GLU:OE1	1:D:463:GLU:N	2.51	0.44
1:D:439:THR:HG23	1:D:544:GLY:HA3	2.00	0.44
1:C:553:SER:HA	1:C:577:VAL:HG11	2.00	0.44
1:D:475:PHE:CG	1:D:476:GLU:N	2.86	0.44
1:C:436:VAL:HB	1:C:545:ILE:HD12	1.99	0.44
1:A:482:ALA:C	1:A:484:LYS:N	2.70	0.43
1:C:520:SER:OG	1:C:523:GLN:HG3	2.18	0.43
1:A:439:THR:HG23	1:A:544:GLY:HA3	2.00	0.43
1:A:520:SER:OG	1:A:523:GLN:HG3	2.19	0.43
1:C:409:ASP:OD2	1:C:488:THR:CG2	2.65	0.42
1:A:539:CYS:SG	1:A:539:CYS:O	2.77	0.42
1:B:536:ILE:HD11	1:B:562:LEU:HD11	2.01	0.42
1:B:395:ASN:CB	1:D:608:THR:O	2.67	0.42
1:C:536:ILE:HD11	1:C:562:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:HD3	1:A:472:PRO:HA	2.01	0.42
1:A:615:PHE:HZ	1:A:617:TRP:HB2	1.82	0.42
1:C:616:ASN:HD21	1:C:618:ARG:HB2	1.85	0.42
1:C:620:TRP:CE3	1:C:620:TRP:HA	2.55	0.42
1:A:471:GLU:O	1:A:474:ILE:HG12	2.19	0.42
1:B:553:SER:HA	1:B:577:VAL:HG11	2.01	0.42
1:A:390:TYR:O	1:A:392:PRO:HD3	2.20	0.41
1:D:412:ASN:HB2	1:D:488:THR:HG21	2.02	0.41
1:A:591:ASN:HD22	1:A:596:LYS:NZ	2.17	0.41
1:B:476:GLU:HG2	1:B:481:GLU:OE2	2.20	0.41
1:B:582:SER:N	1:D:612:ASN:HD21	2.18	0.41
1:B:550:SER:OG	1:B:551:HIS:N	2.51	0.41
1:A:516:MET:C	1:A:518:ALA:H	2.22	0.41
1:C:516:MET:C	1:C:518:ALA:H	2.23	0.41
1:A:439:THR:CG2	1:A:544:GLY:HA3	2.50	0.41
1:C:512:ARG:H	1:C:512:ARG:HG2	1.65	0.41
1:D:367:GLY:HA2	1:D:582:SER:HB3	2.01	0.41
1:B:568:ARG:NH2	1:D:621:ILE:HG23	2.36	0.41
1:A:429:GLU:CD	1:C:398:ARG:HE	2.23	0.41
1:A:593:GLU:HG3	1:A:593:GLU:H	1.68	0.41
1:D:384:THR:OG1	1:D:386:ASP:HB3	2.21	0.41
1:D:441:VAL:O	1:D:441:VAL:HG23	2.20	0.41
1:B:516:MET:C	1:B:518:ALA:H	2.23	0.41
1:A:498:ALA:O	1:A:499:ASN:HB3	2.20	0.41
1:B:439:THR:CG2	1:B:544:GLY:HA3	2.51	0.40
1:B:582:SER:H	1:D:612:ASN:HD21	1.67	0.40
1:A:484:LYS:HD3	1:D:483:SER:N	2.35	0.40
1:D:516:MET:C	1:D:518:ALA:H	2.24	0.40
1:C:406:GLY:C	1:C:408:LYS:H	2.24	0.40
1:D:553:SER:HB2	1:D:573:PHE:HZ	1.85	0.40
1:C:498:ALA:O	1:C:499:ASN:HB3	2.21	0.40
1:D:498:ALA:O	1:D:499:ASN:HB3	2.21	0.40

There are no symmetry-related clashes.

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	265/273 (97%)	242 (91%)	18 (7%)	5 (2%)	10	30
1	B	261/273 (96%)	244 (94%)	17 (6%)	0	100	100
1	C	262/273 (96%)	240 (92%)	15 (6%)	7 (3%)	6	20
1	D	263/273 (96%)	248 (94%)	8 (3%)	7 (3%)	6	20
All	All	1051/1092 (96%)	974 (93%)	58 (6%)	19 (2%)	11	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	405	ASN
1	D	620	TRP
1	C	386	ASP
1	C	619	ASN
1	C	620	TRP
1	D	386	ASP
1	D	483	SER
1	D	594	ASP
1	A	593	GLU
1	A	483	SER
1	A	594	ASP
1	D	593	GLU
1	D	499	ASN
1	A	486	THR
1	C	499	ASN
1	A	517	PRO
1	C	517	PRO
1	D	517	PRO
1	C	407	ILE

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	233/237 (98%)	221 (95%)	12 (5%)	29	61
1	B	230/237 (97%)	215 (94%)	15 (6%)	21	49
1	C	231/237 (98%)	217 (94%)	14 (6%)	23	53
1	D	232/237 (98%)	222 (96%)	10 (4%)	35	69
All	All	926/948 (98%)	875 (94%)	51 (6%)	27	58

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ARG
1	A	370	VAL
1	A	379	LEU
1	A	398	ARG
1	A	409	ASP
1	A	422	PHE
1	A	441	VAL
1	A	460	LEU
1	A	484	LYS
1	A	547	LEU
1	A	593	GLU
1	A	605	LYS
1	B	365	ARG
1	B	370	VAL
1	B	379	LEU
1	B	398	ARG
1	B	409	ASP
1	B	441	VAL
1	B	460	LEU
1	B	486	THR
1	B	487	LEU
1	B	488	THR
1	B	512	ARG
1	B	547	LEU
1	B	593	GLU
1	B	605	LYS
1	B	620	TRP
1	C	365	ARG
1	C	370	VAL
1	C	379	LEU
1	C	398	ARG
1	C	407	ILE
1	C	409	ASP

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Mol	Chain	Res	Type
1	C	422	PHE
1	C	460	LEU
1	C	488	THR
1	C	512	ARG
1	C	593	GLU
1	C	594	ASP
1	C	605	LYS
1	C	620	TRP
1	D	370	VAL
1	D	379	LEU
1	D	398	ARG
1	D	407	ILE
1	D	409	ASP
1	D	460	LEU
1	D	483	SER
1	D	512	ARG
1	D	547	LEU
1	D	605	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	A	612	ASN
1	A	616	ASN
1	B	612	ASN
1	C	601	ASN
1	C	612	ASN
1	D	405	ASN
1	D	612	ASN
1	D	616	ASN
1	D	619	ASN

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 carbohydrates 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	A	1	-	4,4,4	0.28	0	6,6,6	0.31	0
2	PO4	C	3	-	4,4,4	0.39	0	6,6,6	0.28	0
2	PO4	D	4	-	0,3,4	0.00	-	0,3,6	0.00	-

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	1	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3	-	-	0/0/0/0	0/0/0/0
2	PO4	D	4	-	-	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.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	267/273 (97%)	0.34	15 (5%)	28	20	31, 62, 90, 107	0
1	B	263/273 (96%)	0.70	30 (11%)	7	4	31, 62, 83, 105	4 (1%)
1	C	264/273 (96%)	1.09	44 (16%)	2	1	31, 62, 83, 100	6 (2%)
1	D	265/273 (97%)	0.44	17 (6%)	23	16	31, 62, 85, 114	0
All	All	1059/1092 (96%)	0.64	106 (10%)	9	5	31, 62, 86, 114	10 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	SER	19.3
1	C	481	GLU	17.1
1	C	484	LYS	15.4
1	C	485	ALA	14.5
1	C	482	ALA	13.8
1	C	483	SER	13.6
1	C	480	TRP	12.8
1	D	486	THR	6.7
1	D	616	ASN	6.7
1	B	482	ALA	6.5
1	C	515	LEU	5.8
1	B	617	TRP	5.5
1	C	574	ALA	5.5
1	B	386	ASP	5.5
1	B	540	PRO	5.5
1	A	618	ARG	5.5
1	B	484	LYS	5.4
1	B	620	TRP	5.3
1	B	485	ALA	5.2
1	A	485	ALA	5.1
1	B	573	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	573	PHE	5.1
1	C	540	PRO	4.9
1	C	385	ALA	4.9
1	D	620	TRP	4.8
1	D	487	LEU	4.6
1	B	385	ALA	4.5
1	C	570	CYS	4.5
1	D	617	TRP	4.1
1	C	528	CYS	4.1
1	B	571	GLY	4.0
1	C	577	VAL	3.9
1	C	621	ILE	3.9
1	C	386	ASP	3.9
1	C	377	SER	3.8
1	C	387	GLY	3.7
1	B	387	GLY	3.6
1	A	617	TRP	3.6
1	C	617	TRP	3.5
1	B	384	THR	3.5
1	C	620	TRP	3.5
1	D	615	PHE	3.4
1	D	619	ASN	3.4
1	A	385	ALA	3.3
1	B	543	MET	3.3
1	C	576	LEU	3.2
1	C	578	ARG	3.2
1	C	478	MET	3.2
1	D	402	ARG	3.2
1	D	621	ILE	3.2
1	A	386	ASP	3.1
1	B	568	ARG	3.1
1	D	618	ARG	3.0
1	B	613	SER	3.0
1	A	357	SER	3.0
1	A	592	ARG	3.0
1	A	615	PHE	3.0
1	C	513	CYS	2.9
1	C	380	GLN	2.9
1	B	574	ALA	2.8
1	B	570	CYS	2.8
1	C	516	MET	2.8
1	B	530	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	615	PHE	2.8
1	B	619	ASN	2.8
1	D	485	ALA	2.7
1	C	575	GLN	2.7
1	B	388	LYS	2.7
1	A	486	THR	2.7
1	B	481	GLU	2.6
1	C	541	GLN	2.6
1	D	386	ASP	2.6
1	C	507	ARG	2.6
1	C	410	PHE	2.6
1	C	518	ALA	2.6
1	A	620	TRP	2.5
1	C	465	LYS	2.4
1	A	493	GLU	2.4
1	A	616	ASN	2.3
1	C	358	ARG	2.3
1	C	525	VAL	2.3
1	C	521	TYR	2.3
1	A	356	ILE	2.3
1	C	488	THR	2.3
1	A	483	SER	2.3
1	C	520	SER	2.3
1	C	539	CYS	2.3
1	B	406	GLY	2.2
1	C	567	PRO	2.2
1	B	480	TRP	2.2
1	B	564	GLY	2.2
1	D	578	ARG	2.2
1	C	562	LEU	2.2
1	C	514	SER	2.2
1	B	592	ARG	2.1
1	B	569	GLU	2.1
1	C	384	THR	2.1
1	D	465	LYS	2.1
1	D	435	GLY	2.1
1	D	576	LEU	2.1
1	B	577	VAL	2.1
1	C	476	GLU	2.0
1	A	407	ILE	2.0
1	B	567	PRO	2.0
1	C	510	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	506	TYR	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($Å^2$)	Q<0.9
2	PO4	A	1	5/5	0.91	0.19	0.89	77,78,80,82	0
2	PO4	D	4	4/5	0.91	0.20	0.50	88,90,91,91	0
2	PO4	C	3	5/5	0.78	0.25	-0.20	99,100,101,102	0

6.5 Other polymers (i)

There are no such residues in this entry.