Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:19 am BST

PDB ID	:	3D4I
Title	:	Crystal structure of the 2H-phosphatase domain of Sts-2
Authors	:	Chen, Y.; Carpino, N.; Nassar, N.
Deposited on	:	2008-05-14
Resolution	:	1.95 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 following versions of software and data (see references ①) were used in the production of this report:

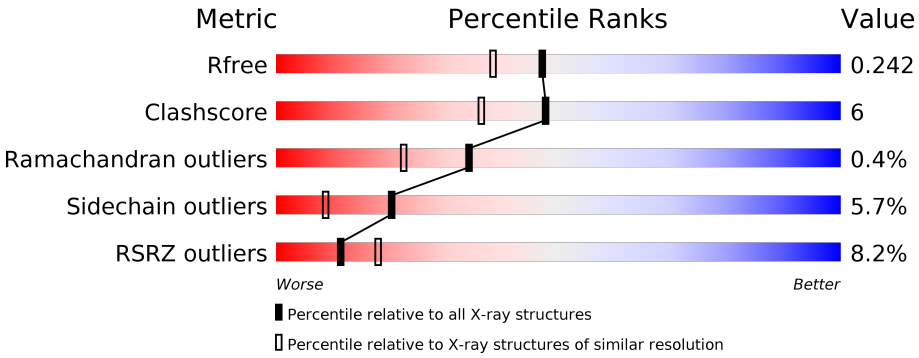
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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 <=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% 85% 13%
1	B	273	13% 77% 18%
1	C	273	7% 84% 11%
1	D	273	7% 81% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8809 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	273	Total	C	N	O	S	0	7	0
			2170	1371	382	400	17			
1	B	264	Total	C	N	O	S	0	3	0
			2107	1331	378	382	16			
1	C	263	Total	C	N	O	S	0	3	0
			2096	1326	371	383	16			
1	D	265	Total	C	N	O	S	0	3	0
			2112	1335	376	386	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is water.

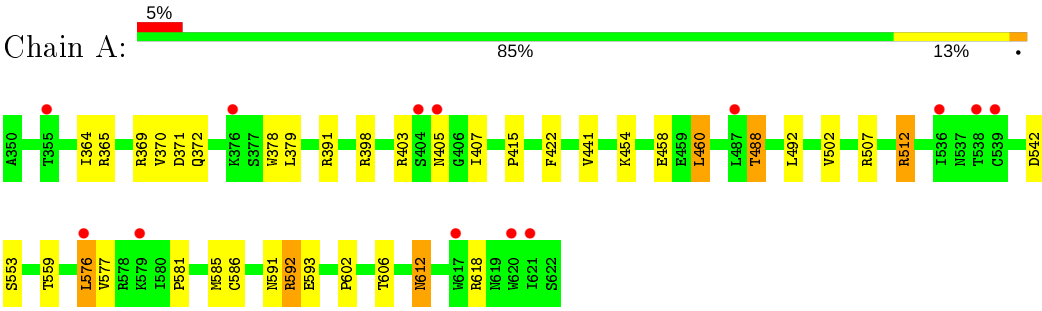
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	105	Total O 105 105	0	0
3	B	54	Total O 54 54	0	0
3	C	89	Total O 89 89	0	0
3	D	75	Total O 75 75	0	0

3 Residue-property plots (i)

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.

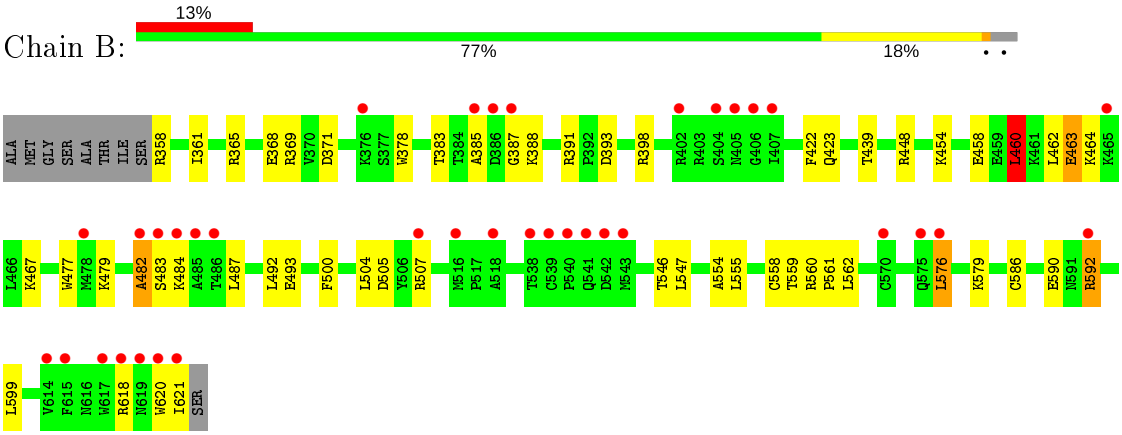
- Molecule 1: Sts-2 protein

Chain A:



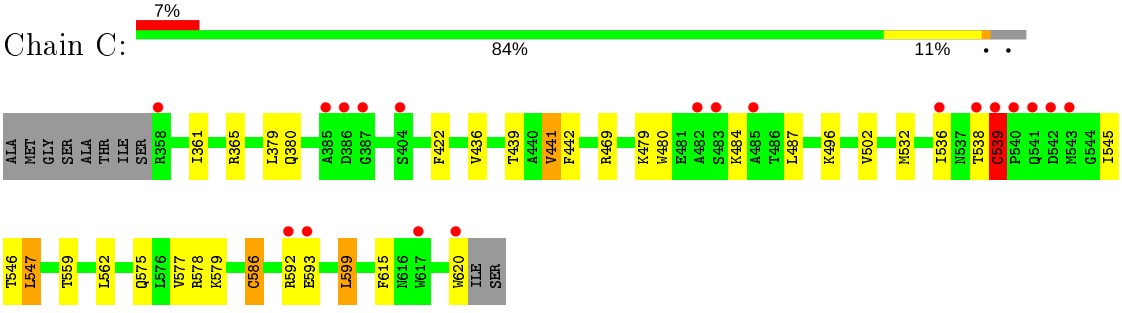
- Molecule 1: Sts-2 protein

Chain B:



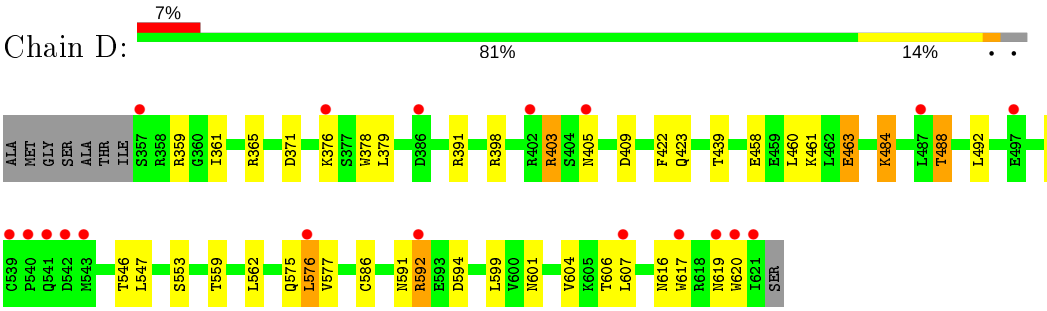
- Molecule 1: Sts-2 protein

Chain C:



- Molecule 1: Sts-2 protein

Chain D:


7%
81%
14%
ALA MET GLY SER ALA THR ILE S357 R358 R359 G360 I361 R365 D371 K376 S377 W378 L379 D386 R391 R398 R402 R403 S404 N405 D409 F422 Q423 T439 E458 E459 L460 K461 L462 E463 K484 L487 T488 L492 E497 R507 I536
C539 P540 Q541 D542 N543 T546 L547 S553 T559 L562 Q575 L576 V577 C586 N591 R592 E593 D594 L599 V600 N601 V604 K605 T606 L607 N616 W617 R618 N619 W620 I621 SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.89Å 115.71Å 121.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.19 – 1.95 44.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.19-1.95) 99.7 (44.21-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.00 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.248 0.205 , 0.242	Depositor DCC
R_{free} test set	4009 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8809	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8590e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL

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	0.60	0/2256	0.68	2/3055 (0.1%)
1	B	0.51	0/2172	0.63	1/2941 (0.0%)
1	C	0.63	2/2158 (0.1%)	0.68	0/2924
1	D	0.56	0/2177	0.64	0/2949
All	All	0.58	2/8763 (0.0%)	0.66	3/11869 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	586[A]	CYS	CB-SG	-7.39	1.69	1.82
1	C	586[B]	CYS	CB-SG	-7.39	1.69	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	460	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	460	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	365	ARG	NE-CZ-NH2	-5.31	117.65	120.30

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	2170	0	2168	34	0
1	B	2107	0	2107	34	0
1	C	2096	0	2094	18	0
1	D	2112	0	2110	30	0
2	B	1	0	0	0	0
3	A	105	0	0	3	0
3	B	54	0	0	0	0
3	C	89	0	0	0	0
3	D	75	0	0	1	0
All	All	8809	0	8479	103	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 6.

All (103) 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:D:376:LYS:O	1:D:376:LYS:HD3	1.69	0.93
1:A:585[B]:MET:HE3	1:A:602:PRO:HB3	1.52	0.90
1:A:492:LEU:HD22	1:A:502:VAL:HG11	1.65	0.79
1:A:369:ARG:HG3	1:A:372[B]:GLN:HG3	1.63	0.78
1:A:369:ARG:CG	1:A:372[B]:GLN:HG3	2.13	0.77
1:C:532:MET:O	1:C:536:ILE:HG12	1.87	0.75
1:B:586[A]:CYS:SG	1:B:599:LEU:HD21	2.32	0.70
1:A:512:ARG:HD2	3:A:128:HOH:O	1.90	0.70
1:C:586[B]:CYS:SG	1:C:599:LEU:HD21	2.33	0.69
1:B:393:ASP:OD2	1:D:606:THR:HG23	1.93	0.68
1:D:458:GLU:HA	1:D:463:GLU:CG	2.24	0.67
1:A:543[B]:MET:CE	1:A:592:ARG:HH21	2.06	0.67
1:A:403:ARG:NH2	1:A:488:THR:O	2.28	0.67
1:B:482:ALA:O	1:B:483:SER:OG	2.14	0.65
1:A:543[B]:MET:HE1	1:A:592:ARG:HH21	1.62	0.65
1:B:586[B]:CYS:SG	1:D:617:TRP:CG	2.89	0.64
1:D:403:ARG:NH2	1:D:488:THR:O	2.30	0.64
1:D:458:GLU:HG2	1:D:463:GLU:HG2	1.79	0.63
1:C:441:VAL:HB	1:C:547:LEU:HB2	1.81	0.63
1:D:391:ARG:HD2	1:D:398:ARG:HA	1.81	0.62
1:C:578:ARG:HG3	1:C:579:LYS:HG3	1.82	0.61
1:D:484:LYS:HD2	1:D:484:LYS:H	1.67	0.59
1:D:616:ASN:HD22	1:D:619:ASN:H	1.50	0.58
1:D:592:ARG:H	1:D:592:ARG:HD2	1.69	0.58
1:D:458:GLU:HA	1:D:463:GLU:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:LYS:HD2	1:D:484:LYS:N	2.20	0.57
1:B:618:ARG:NH2	1:D:601:ASN:HD21	2.04	0.56
1:A:586:CYS:HG	1:C:620:TRP:HH2	1.50	0.56
1:D:458:GLU:HA	1:D:463:GLU:HG2	1.87	0.56
1:D:361:ILE:HD13	1:D:546:THR:HB	1.89	0.55
1:C:559:THR:HG21	1:C:586[B]:CYS:SG	2.46	0.55
1:C:496:LYS:HE2	1:C:502:VAL:O	2.06	0.55
1:A:369:ARG:HG2	1:A:372[B]:GLN:HG3	1.88	0.54
1:A:585[B]:MET:HE2	3:A:246:HOH:O	2.08	0.54
1:B:482:ALA:HB3	1:B:487:LEU:HB2	1.89	0.53
1:A:581:PRO:HG3	1:C:615:PHE:HB2	1.91	0.53
1:B:458:GLU:HG2	1:B:463:GLU:HG2	1.91	0.53
1:B:454:LYS:HE3	1:B:500:PHE:CE1	2.44	0.53
1:A:370[B]:VAL:HG23	1:A:415:PRO:O	2.09	0.52
1:A:543[B]:MET:HE1	1:A:592:ARG:NH2	2.25	0.52
1:B:555:LEU:HD23	1:B:586[B]:CYS:SG	2.49	0.52
1:A:591:ASN:OD1	1:A:593:GLU:HB2	2.10	0.52
1:A:542:ASP:O	1:A:543[B]:MET:HE2	2.10	0.51
1:B:371:ASP:HB3	1:B:378:TRP:CD1	2.45	0.51
1:A:612:ASN:C	1:A:612:ASN:HD22	2.14	0.51
1:D:484:LYS:CD	1:D:484:LYS:H	2.23	0.51
1:D:559:THR:HG21	1:D:586:CYS:SG	2.50	0.51
1:B:458:GLU:HA	1:B:463:GLU:CG	2.41	0.51
1:D:405:ASN:HB2	1:D:409:ASP:OD2	2.11	0.50
1:D:458:GLU:CG	1:D:463:GLU:HG2	2.41	0.50
1:A:585[B]:MET:HE3	1:A:602:PRO:CB	2.35	0.50
1:A:441:VAL:HB	1:A:547:LEU:HB2	1.92	0.50
1:B:576:LEU:HD23	1:D:620:TRP:CD1	2.47	0.50
1:B:592:ARG:HB2	1:B:592:ARG:CZ	2.41	0.49
1:B:458:GLU:HA	1:B:463:GLU:HG2	1.94	0.49
1:A:606:THR:HG21	1:C:615:PHE:O	2.13	0.49
1:A:559:THR:HG21	1:A:586:CYS:SG	2.53	0.49
1:A:618:ARG:HG2	1:C:599:LEU:HD13	1.95	0.49
1:D:365:ARG:CZ	3:D:22:HOH:O	2.61	0.49
1:D:423:GLN:HG2	1:D:607[A]:LEU:HD21	1.95	0.48
1:B:358:ARG:HD3	1:B:590:GLU:O	2.13	0.48
1:D:359:ARG:NH2	1:D:536:ILE:O	2.45	0.47
1:A:586:CYS:SG	1:C:620:TRP:HH2	2.37	0.47
1:B:460:LEU:O	1:B:462:LEU:HD13	2.15	0.47
1:B:361:ILE:HD13	1:B:546:THR:HB	1.97	0.46
1:B:368:GLU:H	1:B:423:GLN:NE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LYS:HD3	1:C:480:TRP:CD1	2.51	0.46
1:B:559:THR:HG21	1:B:586[A]:CYS:SG	2.55	0.46
1:B:621:ILE:HG22	1:D:599:LEU:HD11	1.96	0.46
1:B:493:GLU:H	1:B:493:GLU:CD	2.17	0.46
1:B:391:ARG:HD2	1:B:398:ARG:HA	1.98	0.46
1:B:368:GLU:H	1:B:423:GLN:HE22	1.62	0.46
1:D:371:ASP:HB3	1:D:378:TRP:CD1	2.50	0.46
1:A:585[B]:MET:CE	1:A:602:PRO:HB3	2.34	0.45
1:A:371:ASP:HB3	1:A:378:TRP:CD1	2.52	0.45
1:B:560:ARG:N	1:B:561:PRO:HD2	2.31	0.45
1:B:369:ARG:HG2	1:B:448:ARG:HD2	1.99	0.45
1:D:361:ILE:HG13	1:D:562:LEU:HD21	1.99	0.44
1:C:575:GLN:O	1:C:578:ARG:HG2	2.17	0.44
1:A:553:SER:HA	1:A:577:VAL:HG11	2.00	0.44
1:C:538:THR:O	1:C:539:CYS:HB2	2.19	0.43
1:C:442:PHE:CE2	1:C:469:ARG:HD2	2.54	0.43
1:B:554:ALA:O	1:B:558:CYS:HB2	2.18	0.43
1:B:385:ALA:C	1:B:387:GLY:H	2.21	0.42
1:B:492:LEU:HD23	1:B:504:LEU:HA	2.00	0.42
1:C:361:ILE:HD13	1:C:546:THR:HB	2.01	0.42
1:D:553:SER:HA	1:D:577:VAL:HG22	2.01	0.42
1:B:460:LEU:HG	1:B:462:LEU:HD22	2.01	0.42
1:B:383:THR:HA	1:B:388:LYS:O	2.20	0.42
1:A:372[A]:GLN:NE2	3:A:80:HOH:O	2.52	0.42
1:A:454:LYS:HE2	1:A:458:GLU:OE2	2.20	0.42
1:B:620:TRP:HB3	1:D:576:LEU:HD11	2.01	0.42
1:B:618:ARG:HH22	1:D:601:ASN:HD21	1.68	0.42
1:B:477:TRP:CZ2	1:B:479:LYS:HD3	2.55	0.41
1:B:454:LYS:HE3	1:B:500:PHE:CD1	2.55	0.41
1:A:576:LEU:HD11	1:C:620:TRP:HB3	2.02	0.41
1:A:369:ARG:HG2	1:A:372[B]:GLN:OE1	2.20	0.41
1:C:436:VAL:HB	1:C:545:ILE:HD12	2.01	0.41
1:D:591:ASN:HB3	1:D:594:ASP:OD1	2.21	0.40
1:A:379:LEU:HD11	1:A:407:ILE:HG12	2.03	0.40
1:A:391:ARG:HD2	1:A:398:ARG:HA	2.03	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	278/273 (102%)	275 (99%)	3 (1%)	0	100 100
1	B	265/273 (97%)	253 (96%)	10 (4%)	2 (1%)	19 9
1	C	264/273 (97%)	255 (97%)	7 (3%)	2 (1%)	19 9
1	D	266/273 (97%)	262 (98%)	4 (2%)	0	100 100
All	All	1073/1092 (98%)	1045 (97%)	24 (2%)	4 (0%)	34 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	ALA
1	B	484	LYS
1	C	539	CYS
1	C	484	LYS

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	244/237 (103%)	235 (96%)	9 (4%)	34 22
1	B	234/237 (99%)	220 (94%)	14 (6%)	19 8
1	C	233/237 (98%)	219 (94%)	14 (6%)	19 8
1	D	235/237 (99%)	219 (93%)	16 (7%)	16 5
All	All	946/948 (100%)	893 (94%)	53 (6%)	20 9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ASN
1	A	422	PHE
1	A	460	LEU
1	A	488	THR
1	A	507	ARG
1	A	512	ARG
1	A	576	LEU
1	A	592	ARG
1	A	612	ASN
1	B	365	ARG
1	B	422	PHE
1	B	439	THR
1	B	460	LEU
1	B	463	GLU
1	B	464	LYS
1	B	467	LYS
1	B	505	ASP
1	B	507	ARG
1	B	547	LEU
1	B	562	LEU
1	B	576	LEU
1	B	579	LYS
1	B	592	ARG
1	C	365	ARG
1	C	379	LEU
1	C	380	GLN
1	C	422	PHE
1	C	439	THR
1	C	441	VAL
1	C	487	LEU
1	C	539	CYS
1	C	547	LEU
1	C	562	LEU
1	C	577	VAL
1	C	592	ARG
1	C	593	GLU
1	C	599	LEU
1	D	379	LEU
1	D	403	ARG
1	D	422	PHE
1	D	439	THR
1	D	460	LEU

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Mol	Chain	Res	Type
1	D	461	LYS
1	D	463	GLU
1	D	484	LYS
1	D	488	THR
1	D	492	LEU
1	D	507	ARG
1	D	547	LEU
1	D	575	GLN
1	D	576	LEU
1	D	592	ARG
1	D	604	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	GLN
1	A	612	ASN
1	B	423	GLN
1	C	380	GLN
1	D	601	ASN
1	D	612	ASN
1	D	616	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	273/273 (100%)	0.48	13 (4%)	30	40	13, 24, 42, 49	0
1	B	264/273 (96%)	0.88	36 (13%)	3	4	18, 31, 47, 58	4 (1%)
1	C	263/273 (96%)	0.48	19 (7%)	15	23	13, 26, 42, 59	0
1	D	265/273 (97%)	0.46	19 (7%)	15	23	16, 26, 46, 60	0
All	All	1065/1092 (97%)	0.57	87 (8%)	11	18	13, 26, 44, 60	4 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	SER	12.8
1	B	485	ALA	11.9
1	B	484	LYS	9.5
1	C	540	PRO	9.4
1	D	620	TRP	8.5
1	C	620	TRP	7.1
1	C	541	GLN	6.7
1	B	543	MET	6.5
1	B	482	ALA	6.3
1	B	539	CYS	6.2
1	B	620	TRP	6.0
1	C	482	ALA	5.7
1	A	404	SER	5.4
1	B	385	ALA	5.3
1	B	486	THR	5.1
1	D	541	GLN	5.1
1	C	385	ALA	4.6
1	C	386	ASP	4.6
1	D	539	CYS	4.6
1	D	619	ASN	4.6
1	A	538	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	483	SER	4.4
1	C	543	MET	4.3
1	D	542	ASP	4.2
1	A	405	ASN	4.2
1	D	540	PRO	4.2
1	B	386	ASP	4.2
1	C	539	CYS	4.1
1	B	541	GLN	3.9
1	C	358	ARG	3.9
1	B	621	ILE	3.9
1	B	542	ASP	3.8
1	B	518	ALA	3.8
1	B	406	GLY	3.8
1	D	621	ILE	3.7
1	A	487	LEU	3.7
1	C	387	GLY	3.7
1	A	620	TRP	3.6
1	D	487	LEU	3.4
1	C	542	ASP	3.3
1	B	404	SER	3.2
1	C	617	TRP	3.1
1	D	592	ARG	3.1
1	C	593	GLU	3.0
1	B	507	ARG	3.0
1	B	538	THR	2.9
1	A	539	CYS	2.9
1	B	387	GLY	2.9
1	B	540	PRO	2.8
1	D	617	TRP	2.8
1	D	402	ARG	2.8
1	B	576	LEU	2.8
1	B	617	TRP	2.7
1	B	402[A]	ARG	2.7
1	A	536	ILE	2.7
1	C	538	THR	2.7
1	D	405	ASN	2.7
1	C	404	SER	2.7
1	A	617	TRP	2.5
1	B	407	ILE	2.4
1	B	614	VAL	2.4
1	D	576	LEU	2.4
1	B	575	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	357	SER	2.4
1	C	536	ILE	2.4
1	B	615	PHE	2.4
1	B	619	ASN	2.4
1	A	576	LEU	2.3
1	A	579	LYS	2.3
1	B	570	CYS	2.3
1	B	478	MET	2.3
1	D	386	ASP	2.3
1	B	516	MET	2.3
1	D	543	MET	2.3
1	B	592	ARG	2.3
1	C	485	ALA	2.3
1	B	376	LYS	2.2
1	A	621	ILE	2.2
1	D	607[A]	LEU	2.2
1	B	405	ASN	2.1
1	C	592	ARG	2.1
1	D	376	LYS	2.1
1	A	355	THR	2.1
1	D	497	GLU	2.1
1	B	618	ARG	2.0
1	A	376	LYS	2.0
1	B	465	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. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
2	CL	B	1	1/1	0.87	0.20	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.