Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 01:53 PM BST

PDB ID	:	6TLC
Title	:	Unphosphorylated human STAT3 in complex with MS3-6 monobody
Authors	:	La Sala, G.; Lau, K.; Reynaud, A.; Pojer, F.; Hantschel, O.
Deposited on	:	2019-12-02
Resolution	:	2.90 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:

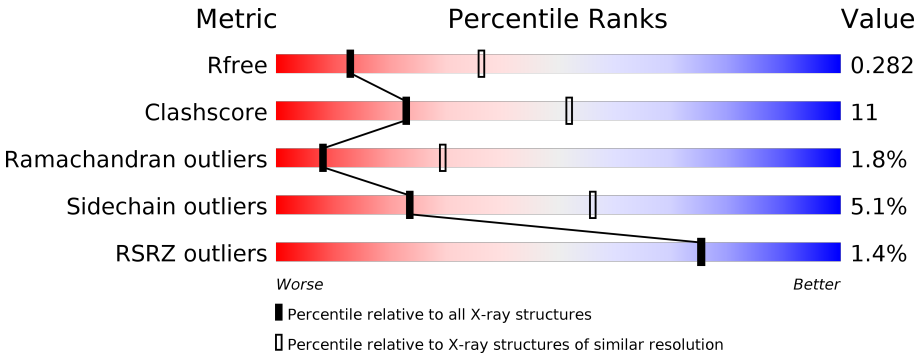
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	598	2% 65% 20% • 11%
1	B	598	% 68% 19% • 11%
2	C	95	66% 32% •
2	D	95	64% 34% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10064 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 Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	535	Total	C	N	O	S	0	0	0
			4318	2755	737	797	29			
1	A	533	Total	C	N	O	S	0	0	0
			4298	2743	731	797	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	125	GLY	-	expression tag	UNP P40763
B	126	SER	-	expression tag	UNP P40763
A	125	GLY	-	expression tag	UNP P40763
A	126	SER	-	expression tag	UNP P40763

- Molecule 2 is a protein called Monobody.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	95	Total	C	N	O	0	0	0
			723	470	107	146			
2	C	95	Total	C	N	O	0	0	0
			723	470	107	146			

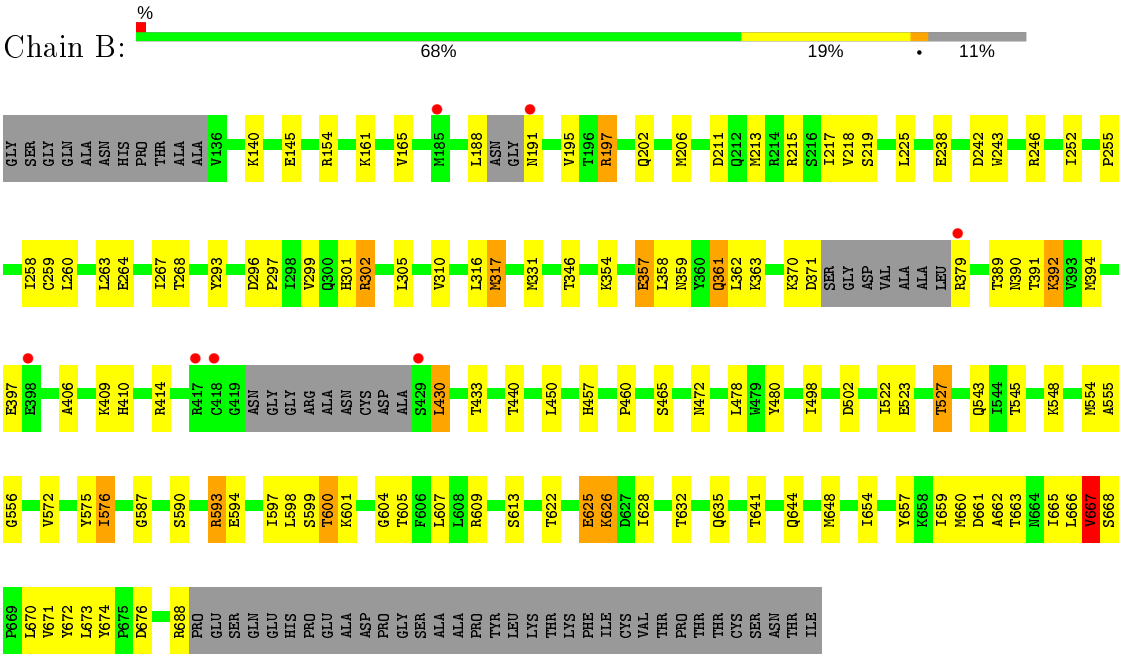
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	A	1	Total	O	0	0
			1	1		

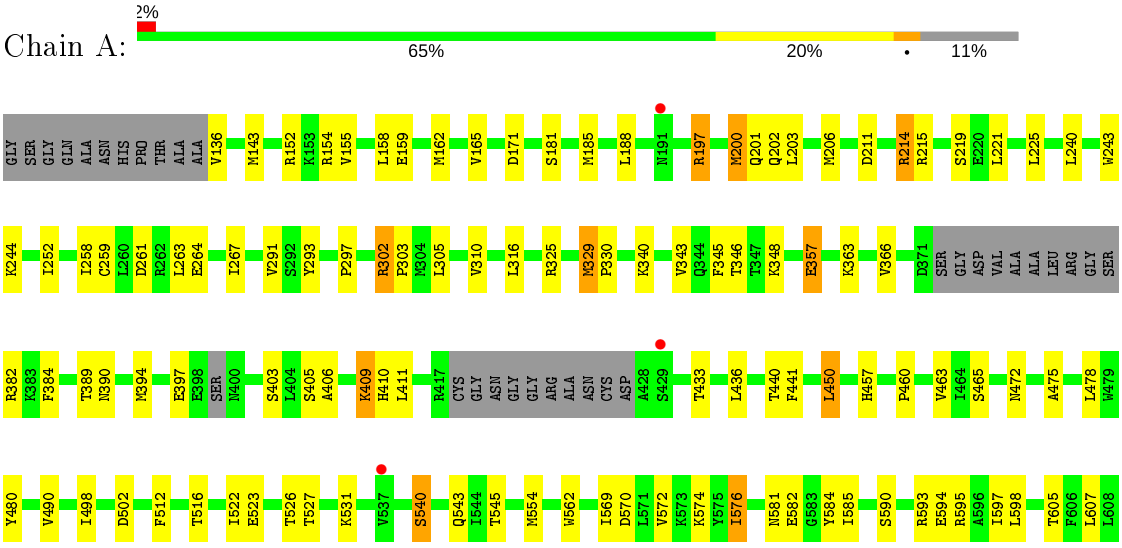
3 Residue-property plots (i)

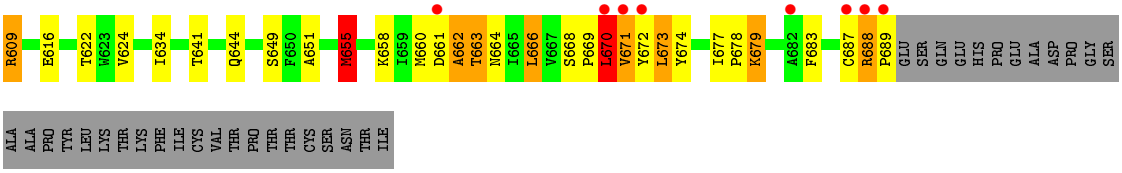
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Signal transducer and activator of transcription 3



- Molecule 1: Signal transducer and activator of transcription 3





- Molecule 2: Monobody

Chain D:

- Molecule 2: Monobody

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.31Å 111.31Å 483.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 2.90 49.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.78-2.90) 99.8 (49.78-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.246 , 0.281 0.250 , 0.282	Depositor DCC
R_{free} test set	3429 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10064	wwPDB-VP
Average B, all atoms (Å^2)	83.0	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 45.49 % 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 1.3119e-04. 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

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	0.72	0/4380	0.94	13/5915 (0.2%)
1	B	0.77	3/4399 (0.1%)	0.97	7/5936 (0.1%)
2	C	0.76	0/746	0.96	0/1028
2	D	0.78	0/746	0.96	2/1028 (0.2%)
All	All	0.75	3/10271 (0.0%)	0.95	22/13907 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	676	ASP	CB-CG	7.09	1.66	1.51
1	B	625	GLU	CG-CD	5.91	1.60	1.51
1	B	625	GLU	CD-OE1	-5.24	1.19	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	625	GLU	OE1-CD-OE2	-8.53	113.06	123.30
1	A	609	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	214	ARG	CG-CD-NE	7.43	127.41	111.80
1	B	676	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	302	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	317	MET	CG-SD-CE	-6.13	90.39	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	607	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	670	LEU	CB-CG-CD2	5.76	120.80	111.00
1	A	261	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	409	LYS	N-CA-C	-5.56	95.99	111.00
1	B	302	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	D	92	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	D	5	PRO	CA-N-CD	-5.40	103.94	111.50
1	A	325	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	609	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	655	MET	CA-CB-CG	5.37	122.42	113.30
1	B	317	MET	CA-CB-CG	-5.26	104.36	113.30
1	A	200	MET	CA-CB-CG	-5.20	104.46	113.30
1	A	261	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	667	VAL	N-CA-C	-5.12	97.16	111.00
1	A	390	ASN	N-CA-CB	-5.09	101.43	110.60
1	B	390	ASN	N-CA-CB	-5.05	101.52	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	THR	Peptide
1	A	673	LEU	Peptide
1	B	389	THR	Peptide
1	B	673	LEU	Peptide
2	D	42	ASN	Peptide

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	4298	0	4329	105	0
1	B	4318	0	4362	70	0
2	C	723	0	702	25	1
2	D	723	0	702	34	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10064	0	10095	229	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (229) 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:197:ARG:HH11	1:A:201:GLN:HB2	1.09	1.18
1:A:197:ARG:HH11	1:A:201:GLN:CB	1.63	1.11
2:C:4:VAL:HG13	2:C:5:PRO:HD3	1.30	1.10
1:A:197:ARG:NH1	1:A:201:GLN:HB2	1.75	1.01
1:B:359:ASN:O	1:B:361:GLN:NE2	1.93	1.00
1:A:197:ARG:NH1	1:A:201:GLN:CB	2.24	1.00
2:C:4:VAL:HG21	2:C:74:ALA:HB3	1.49	0.93
2:C:4:VAL:HG13	2:C:5:PRO:CD	2.01	0.90
2:D:4:VAL:HG12	2:D:5:PRO:HD3	1.53	0.90
2:D:4:VAL:CG1	2:D:5:PRO:HD3	2.03	0.87
2:C:4:VAL:HG21	2:C:74:ALA:CB	2.04	0.85
1:A:655:MET:HA	1:A:679:LYS:HZ3	1.41	0.85
1:B:659:ILE:O	1:B:666:LEU:HD22	1.79	0.83
2:D:4:VAL:HG12	2:D:5:PRO:CD	2.10	0.81
1:A:660:MET:HE2	1:A:664:ASN:HA	1.63	0.80
1:A:641:THR:HG22	1:A:644:GLN:OE1	1.80	0.79
1:B:641:THR:HG22	1:B:644:GLN:OE1	1.83	0.78
1:A:669:PRO:O	1:A:671:VAL:N	2.18	0.76
1:A:663:THR:OG1	1:A:664:ASN:N	2.17	0.76
1:A:655:MET:HG3	1:A:679:LYS:HE2	1.70	0.74
1:A:679:LYS:HD3	1:A:679:LYS:C	2.08	0.74
1:A:346:THR:HG22	1:A:409:LYS:HA	1.68	0.74
1:A:197:ARG:NH1	1:A:201:GLN:CA	2.52	0.73
1:A:197:ARG:HH11	1:A:201:GLN:CG	2.00	0.73
1:A:655:MET:HA	1:A:679:LYS:NZ	2.05	0.71
2:D:4:VAL:HG13	2:D:74:ALA:HB3	1.71	0.70
2:D:4:VAL:HG13	2:D:74:ALA:CB	2.21	0.70
1:A:440:THR:HG22	1:A:457:HIS:HB3	1.74	0.69
2:D:4:VAL:CB	2:D:5:PRO:HD3	2.22	0.69
1:A:264:GLU:OE2	1:A:403:SER:OG	2.12	0.68
1:B:598:LEU:HD11	1:B:607:LEU:HD22	1.75	0.68
2:C:4:VAL:CG1	2:C:5:PRO:HD3	2.17	0.67
1:A:641:THR:CG2	1:A:644:GLN:OE1	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:THR:HG22	1:B:457:HIS:HB3	1.75	0.67
2:D:19:LEU:CD1	2:D:58:THR:HG22	2.25	0.66
2:D:19:LEU:HD13	2:D:58:THR:HG22	1.77	0.65
1:A:687:CYS:SG	1:A:688:ARG:N	2.69	0.65
1:B:268:THR:HG22	1:B:354:LYS:H	1.61	0.65
1:B:202:GLN:O	1:B:206:MET:HG3	1.97	0.64
1:B:600:THR:HG23	1:B:601:LYS:HD2	1.78	0.64
1:A:512:PHE:O	1:A:516:THR:HG23	1.98	0.64
1:B:625:GLU:OE2	1:B:635:GLN:OE1	2.15	0.63
1:A:593:ARG:O	1:A:597:ILE:HG22	2.00	0.62
1:B:605:THR:HG22	1:B:672:TYR:HB2	1.82	0.62
1:B:659:ILE:O	1:B:666:LEU:CD2	2.47	0.62
2:D:78:TYR:HB3	2:D:79:PRO:HD3	1.81	0.61
1:A:576:ILE:HD12	1:A:585:ILE:CD1	2.32	0.60
1:A:670:LEU:O	1:A:670:LEU:HD23	2.02	0.59
2:D:4:VAL:HB	2:D:5:PRO:HD3	1.82	0.58
1:B:296:ASP:O	1:B:299:VAL:HG12	2.03	0.58
1:B:666:LEU:O	1:B:667:VAL:HG13	2.03	0.58
1:A:214:ARG:NH1	1:A:291:VAL:O	2.37	0.58
2:C:4:VAL:HB	2:C:84:PRO:HG2	1.85	0.58
2:C:28:THR:OG1	2:C:78:TYR:HB3	2.03	0.58
1:A:211:ASP:OD1	1:A:215:ARG:NH2	2.37	0.58
1:A:594:GLU:OE2	1:A:609:ARG:NH1	2.36	0.58
1:A:679:LYS:CD	1:A:679:LYS:C	2.73	0.58
1:B:597:ILE:HG12	1:B:674:TYR:CE1	2.39	0.57
2:C:0:SER:O	2:C:1:VAL:HG12	2.03	0.57
1:A:197:ARG:NH1	1:A:201:GLN:CG	2.65	0.57
1:A:660:MET:HE2	1:A:664:ASN:CA	2.33	0.57
1:B:397:GLU:CB	1:A:159:GLU:OE2	2.52	0.57
1:B:264:GLU:O	1:B:268:THR:HG23	2.05	0.57
1:A:197:ARG:NH1	1:A:201:GLN:HA	2.20	0.57
2:D:33:HIS:CD2	2:D:49:THR:HG22	2.39	0.57
2:D:3:SER:OG	2:D:5:PRO:O	2.23	0.57
1:B:140:LYS:NZ	1:B:238:GLU:OE1	2.23	0.57
1:B:346:THR:HG22	1:B:409:LYS:HA	1.86	0.57
1:B:659:ILE:H	1:B:666:LEU:CD2	2.18	0.56
1:B:211:ASP:OD1	1:B:215:ARG:NH2	2.38	0.56
1:B:626:LYS:HE2	1:B:632:THR:CG2	2.34	0.56
1:A:498:ILE:HD13	1:A:543:GLN:HB2	1.88	0.56
1:B:575:TYR:C	1:B:576:ILE:HG22	2.25	0.56
1:A:677:ILE:HG22	1:A:678:PRO:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:THR:HG23	1:B:548:LYS:H	1.71	0.56
1:B:660:MET:HE1	1:B:663:THR:O	2.06	0.56
1:A:197:ARG:HH12	1:A:201:GLN:HA	1.70	0.55
2:C:34:ILE:HD13	2:C:72:VAL:HG22	1.88	0.55
1:A:605:THR:HA	1:A:672:TYR:O	2.06	0.55
1:B:661:ASP:O	1:B:663:THR:N	2.41	0.54
1:A:605:THR:HG22	1:A:672:TYR:HB2	1.89	0.54
1:B:523:GLU:O	1:B:527:THR:HG23	2.08	0.54
1:B:594:GLU:OE2	1:B:609:ARG:NH1	2.40	0.54
1:A:267:ILE:HG23	1:A:316:LEU:HD11	1.88	0.54
1:B:593:ARG:O	1:B:597:ILE:HG22	2.07	0.54
1:B:267:ILE:HG23	1:B:316:LEU:HD11	1.89	0.54
1:B:460:PRO:HG2	1:B:480:TYR:CZ	2.43	0.53
1:A:240:LEU:HA	1:A:263:LEU:HD11	1.91	0.53
2:C:78:TYR:HB3	2:C:79:PRO:HD3	1.89	0.53
2:D:34:ILE:HD13	2:D:72:VAL:HG22	1.90	0.53
2:C:-1:GLY:O	2:C:0:SER:OG	2.23	0.53
1:A:523:GLU:O	1:A:527:THR:HG23	2.09	0.53
1:B:391:THR:O	1:B:392:LYS:HD2	2.09	0.52
1:B:604:GLY:HA3	1:B:671:VAL:HB	1.90	0.52
1:A:384:PHE:CE1	1:A:463:VAL:HG11	2.45	0.52
1:A:679:LYS:HD3	1:A:679:LYS:O	2.09	0.52
1:A:622:THR:HG23	1:A:634:ILE:HG23	1.90	0.52
1:A:512:PHE:O	1:A:516:THR:CG2	2.58	0.52
1:A:661:ASP:O	1:A:662:ALA:O	2.28	0.51
1:B:268:THR:CG2	1:B:354:LYS:H	2.22	0.51
2:C:78:TYR:CD2	2:C:79:PRO:N	2.79	0.51
2:D:4:VAL:HG22	2:D:84:PRO:HG2	1.93	0.51
1:A:651:ALA:O	1:A:655:MET:SD	2.68	0.51
1:A:263:LEU:HD23	1:A:263:LEU:O	2.10	0.51
1:A:366:VAL:HG11	1:A:411:LEU:HD21	1.92	0.50
1:A:663:THR:OG1	1:A:664:ASN:OD1	2.30	0.50
1:A:329:MET:HE2	1:A:343:VAL:HG11	1.93	0.50
1:B:666:LEU:HG	1:B:667:VAL:O	2.12	0.49
2:D:76:VAL:HB	2:D:82:TYR:HB3	1.93	0.49
2:D:28:THR:OG1	2:D:78:TYR:HB3	2.12	0.49
1:A:197:ARG:NH1	1:A:201:GLN:HG3	2.26	0.49
1:A:590:SER:OG	1:A:593:ARG:HB2	2.12	0.49
1:A:329:MET:HE2	1:A:343:VAL:CG1	2.42	0.49
1:B:590:SER:OG	1:B:593:ARG:HB2	2.12	0.49
1:A:582:GLU:OE1	1:A:584:TYR:CE2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:VAL:CG1	2:D:74:ALA:CB	2.89	0.49
1:A:460:PRO:HG2	1:A:480:TYR:CZ	2.48	0.49
1:A:661:ASP:C	1:A:662:ALA:O	2.49	0.49
2:C:76:VAL:HB	2:C:82:TYR:HB3	1.93	0.49
1:A:660:MET:CE	1:A:663:THR:O	2.61	0.48
1:B:211:ASP:HB2	1:B:293:TYR:OH	2.13	0.48
1:A:436:LEU:O	1:A:490:VAL:HG13	2.12	0.48
2:D:20:ILE:O	2:D:56:THR:HB	2.13	0.48
1:A:394:MET:HG2	1:A:406:ALA:HB2	1.96	0.48
1:B:302:ARG:HA	1:B:305:LEU:HD12	1.96	0.48
2:C:20:ILE:O	2:C:56:THR:HB	2.13	0.48
1:A:329:MET:HE1	1:A:340:LYS:HB3	1.96	0.48
1:A:671:VAL:HG12	1:A:672:TYR:CD1	2.49	0.48
1:B:394:MET:HG2	1:B:406:ALA:HB2	1.97	0.47
1:A:671:VAL:HG12	1:A:672:TYR:CG	2.49	0.47
2:C:50:VAL:HG11	2:C:57:ALA:HB2	1.96	0.47
2:C:4:VAL:HB	2:C:84:PRO:CG	2.44	0.47
1:A:211:ASP:HB2	1:A:293:TYR:OH	2.15	0.47
1:A:569:ILE:HA	1:A:572:VAL:HG12	1.96	0.47
1:B:498:ILE:HD12	1:B:543:GLN:NE2	2.29	0.47
2:D:4:VAL:HG13	2:D:74:ALA:HB2	1.96	0.47
2:D:7:LYS:HG2	2:D:23:ASP:HB2	1.95	0.47
1:A:673:LEU:HD11	1:A:683:PHE:CZ	2.50	0.46
1:B:165:VAL:HG22	1:B:213:MET:SD	2.55	0.46
1:B:410:HIS:HE1	1:A:171:ASP:OD1	1.98	0.46
1:A:329:MET:CE	1:A:340:LYS:H	2.29	0.46
1:A:658:LYS:HB3	1:A:666:LEU:O	2.16	0.46
2:D:4:VAL:CG1	2:D:74:ALA:HB2	2.46	0.46
1:A:576:ILE:HD12	1:A:585:ILE:HD11	1.96	0.46
1:B:554:MET:O	1:B:556:GLY:N	2.48	0.46
2:C:39:THR:HG22	2:C:69:THR:OG1	2.16	0.46
2:C:78:TYR:CG	2:C:79:PRO:N	2.79	0.46
1:A:671:VAL:O	1:A:679:LYS:HB2	2.16	0.46
1:B:258:ILE:HG22	1:B:259:CYS:O	2.16	0.46
1:B:572:VAL:HA	1:B:576:ILE:HG23	1.97	0.46
1:B:657:TYR:O	1:B:668:SER:HA	2.16	0.46
2:C:1:VAL:HG13	2:C:6:THR:HG22	1.97	0.45
2:D:18:LEU:CD2	2:D:91:TYR:CD2	2.99	0.45
1:A:310:VAL:HG13	1:A:450:LEU:HD21	1.98	0.45
1:A:688:ARG:HB3	1:A:689:PRO:CD	2.46	0.45
2:D:5:PRO:HD2	2:D:87:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG13	1:B:450:LEU:HD21	1.99	0.45
2:D:78:TYR:CB	2:D:79:PRO:HD3	2.45	0.45
1:A:185:MET:O	1:A:188:LEU:HB3	2.17	0.45
1:A:366:VAL:HG23	1:A:441:PHE:CD1	2.52	0.44
1:B:225:LEU:HD12	1:B:305:LEU:HD23	1.99	0.44
2:D:18:LEU:CD2	2:D:91:TYR:HD2	2.30	0.44
2:D:4:VAL:CB	2:D:5:PRO:CD	2.92	0.44
1:A:581:ASN:O	1:A:582:GLU:HG2	2.18	0.44
1:B:599:SER:HA	1:B:632:THR:HG21	1.99	0.44
1:B:665:ILE:O	1:B:667:VAL:N	2.51	0.44
2:D:4:VAL:HB	2:D:5:PRO:CD	2.47	0.44
1:A:302:ARG:HA	1:A:305:LEU:HD12	1.99	0.44
1:A:348:LYS:HE2	1:A:405:SER:HB3	1.98	0.44
1:B:242:ASP:HB3	1:B:246:ARG:NH2	2.32	0.44
2:D:18:LEU:HD21	2:D:91:TYR:HD2	1.83	0.44
1:A:225:LEU:HD12	1:A:305:LEU:HD23	2.00	0.43
1:B:161:LYS:HB3	1:B:217:ILE:HD11	1.99	0.43
1:A:598:LEU:HD13	1:A:624:VAL:HG23	2.00	0.43
1:B:575:TYR:O	1:B:576:ILE:HG22	2.18	0.43
1:A:215:ARG:CZ	1:A:297:PRO:HG3	2.48	0.43
1:A:366:VAL:HG23	1:A:441:PHE:CE1	2.53	0.43
1:A:433:THR:HG21	1:A:472:ASN:HB2	2.00	0.43
1:B:607:LEU:CD2	1:B:622:THR:HB	2.48	0.43
1:B:605:THR:HA	1:B:672:TYR:O	2.18	0.43
2:D:10:VAL:HG11	2:D:18:LEU:HD22	2.00	0.43
1:A:202:GLN:O	1:A:206:MET:HG2	2.19	0.43
1:A:410:HIS:C	1:A:411:LEU:HD12	2.40	0.43
1:B:252:ILE:HB	1:B:478:LEU:HD23	2.01	0.43
1:A:593:ARG:O	1:A:597:ILE:CG2	2.67	0.43
1:A:594:GLU:OE1	1:A:609:ARG:NH1	2.52	0.43
1:B:218:VAL:HG11	1:B:301:HIS:HB2	2.01	0.43
2:C:39:THR:HG23	2:C:67:ASP:O	2.19	0.43
2:C:4:VAL:HG11	2:C:74:ALA:N	2.34	0.42
2:D:18:LEU:HD22	2:D:91:TYR:CD2	2.54	0.42
1:A:252:ILE:HB	1:A:478:LEU:HD23	2.01	0.42
1:A:522:ILE:O	1:A:526:THR:HG22	2.19	0.42
1:A:595:ARG:CB	1:A:634:ILE:HD11	2.49	0.42
2:D:66:VAL:HG13	2:D:68:TYR:CE2	2.54	0.42
1:A:329:MET:HE1	1:A:340:LYS:H	1.85	0.42
1:A:597:ILE:HG12	1:A:674:TYR:CE1	2.54	0.42
1:B:498:ILE:HD12	1:B:543:GLN:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HA	2:C:33:HIS:CE1	2.55	0.42
2:D:19:LEU:HD12	2:D:58:THR:HG22	1.98	0.42
1:B:414:ARG:NH2	1:A:181:SER:OG	2.53	0.41
1:B:654:ILE:HG23	1:B:670:LEU:HD12	2.02	0.41
2:D:82:TYR:O	2:D:83:PHE:HB2	2.20	0.41
1:A:136:VAL:O	1:A:136:VAL:HG23	2.20	0.41
1:A:475:ALA:HB2	1:A:562:TRP:CD1	2.54	0.41
1:B:654:ILE:HG23	1:B:670:LEU:CD1	2.50	0.41
1:A:330:PRO:HD3	1:A:345:PHE:HA	2.02	0.41
1:A:570:ASP:O	1:A:574:LYS:HG3	2.20	0.41
1:B:243:TRP:CZ2	1:B:260:LEU:HD11	2.55	0.41
1:B:433:THR:HG21	1:B:472:ASN:HB2	2.02	0.41
1:B:576:ILE:O	1:B:576:ILE:CG1	2.68	0.41
2:D:19:LEU:HD13	2:D:58:THR:CG2	2.49	0.41
1:A:158:LEU:HD13	1:A:221:LEU:CD2	2.50	0.41
1:A:670:LEU:CD2	1:A:670:LEU:O	2.68	0.41
1:B:195:VAL:CG2	2:C:49:THR:HG21	2.51	0.41
2:C:82:TYR:O	2:C:83:PHE:HB2	2.21	0.41
1:A:243:TRP:HZ3	1:A:244:LYS:HD3	1.86	0.41
1:A:302:ARG:N	1:A:303:PRO:CD	2.83	0.41
1:B:522:ILE:HD12	1:B:522:ILE:H	1.86	0.41
1:A:158:LEU:HD13	1:A:221:LEU:HD23	2.03	0.41
1:A:152:ARG:O	1:A:155:VAL:HG12	2.20	0.41
1:A:162:MET:HA	1:A:165:VAL:HG12	2.02	0.40
1:A:660:MET:CE	1:A:664:ASN:HA	2.44	0.40
1:A:594:GLU:CD	1:A:609:ARG:HH11	2.24	0.40
1:B:215:ARG:CZ	1:B:297:PRO:HG3	2.50	0.40
1:B:358:LEU:HB3	1:B:362:LEU:HD11	2.04	0.40
2:C:4:VAL:HG21	2:C:74:ALA:HB2	1.96	0.40
1:A:531:LYS:HD3	1:A:554:MET:HE2	2.04	0.40
1:B:370:LYS:O	1:B:371:ASP:HB2	2.22	0.40
1:B:590:SER:O	1:B:594:GLU:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ARG:O	2:C:0:SER:OG[1_655]	1.78	0.42

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	525/598 (88%)	492 (94%)	22 (4%)	11 (2%)	7 26
1	B	527/598 (88%)	498 (94%)	21 (4%)	8 (2%)	10 34
2	C	93/95 (98%)	81 (87%)	9 (10%)	3 (3%)	4 16
2	D	93/95 (98%)	84 (90%)	9 (10%)	0	100 100
All	All	1238/1386 (89%)	1155 (93%)	61 (5%)	22 (2%)	8 29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO
1	B	667	VAL
1	A	258	ILE
1	A	259	CYS
1	A	662	ALA
1	A	670	LEU
2	C	0	SER
2	C	1	VAL
1	B	357	GLU
1	B	587	GLY
1	B	662	ALA
1	A	357	GLU
1	A	688	ARG
1	B	555	ALA
1	A	663	THR
1	A	671	VAL
1	A	397	GLU
1	B	430	LEU
1	A	540	SER
1	B	576	ILE
1	A	576	ILE
2	C	64	PRO

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	479/536 (89%)	458 (96%)	21 (4%)	28	61
1	B	482/536 (90%)	457 (95%)	25 (5%)	23	55
2	C	82/82 (100%)	76 (93%)	6 (7%)	14	38
2	D	82/82 (100%)	77 (94%)	5 (6%)	18	48
All	All	1125/1236 (91%)	1068 (95%)	57 (5%)	24	56

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	GLU
1	B	154	ARG
1	B	188	LEU
1	B	191	ASN
1	B	197	ARG
1	B	219	SER
1	B	263	LEU
1	B	317	MET
1	B	331	MET
1	B	357	GLU
1	B	361	GLN
1	B	363	LYS
1	B	379	ARG
1	B	392	LYS
1	B	430	LEU
1	B	465	SER
1	B	502	ASP
1	B	527	THR
1	B	593	ARG
1	B	600	THR
1	B	613	SER
1	B	626	LYS
1	B	628	ILE
1	B	648	MET

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Mol	Chain	Res	Type
1	B	688	ARG
1	A	143	MET
1	A	154	ARG
1	A	197	ARG
1	A	200	MET
1	A	203	LEU
1	A	219	SER
1	A	329	MET
1	A	357	GLU
1	A	363	LYS
1	A	382	ARG
1	A	450	LEU
1	A	465	SER
1	A	502	ASP
1	A	540	SER
1	A	545	THR
1	A	616	GLU
1	A	649	SER
1	A	655	MET
1	A	666	LEU
1	A	668	SER
1	A	679	LYS
2	D	21	SER
2	D	43	SER
2	D	53	SER
2	D	55	SER
2	D	80	GLU
2	C	2	SER
2	C	21	SER
2	C	53	SER
2	C	55	SER
2	C	80	GLU
2	C	88	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	205	GLN
1	B	410	HIS
1	B	466	ASN
1	A	160	GLN
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	416	GLN
1	A	466	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	533/598 (89%)	-0.07	11 (2%) 63 61	50, 80, 131, 183	0
1	B	535/598 (89%)	-0.12	7 (1%) 77 77	48, 75, 122, 169	0
2	C	95/95 (100%)	-0.12	0 100 100	60, 86, 118, 135	0
2	D	95/95 (100%)	-0.09	0 100 100	57, 82, 120, 134	0
All	All	1258/1386 (90%)	-0.10	18 (1%) 75 75	48, 78, 128, 183	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	CYS	4.0
1	A	688	ARG	2.9
1	B	417	ARG	2.9
1	B	191	ASN	2.9
1	A	191	ASN	2.7
1	A	689	PRO	2.6
1	A	661	ASP	2.5
1	A	672	TYR	2.4
1	A	537	VAL	2.4
1	B	429	SER	2.4
1	B	398	GLU	2.3
1	A	671	VAL	2.3
1	A	670	LEU	2.2
1	A	429	SER	2.2
1	A	682	ALA	2.2
1	B	185	MET	2.2
1	B	379	ARG	2.1
1	A	687	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.