



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:29 AM UTC

PDB ID : 6TLC / pdb_00006tlc
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

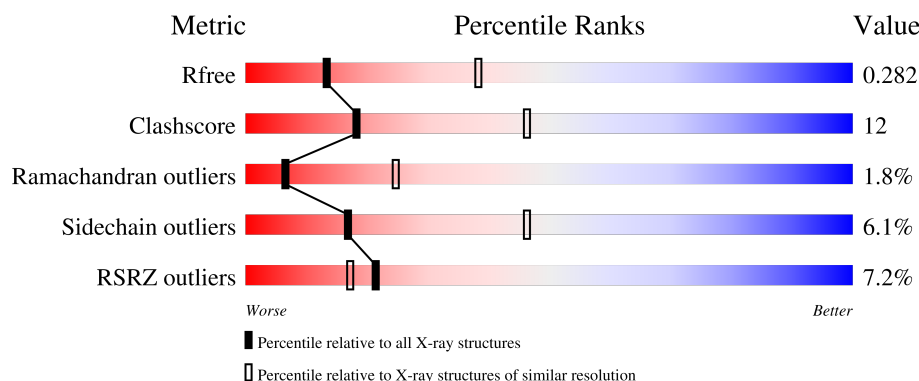
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

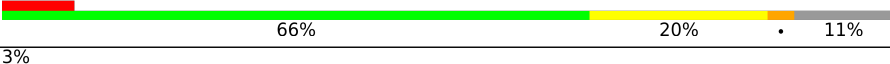
The reported resolution of this entry is 2.90 Å.

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	598	
1	B	598	
2	C	95	
2	D	95	

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:

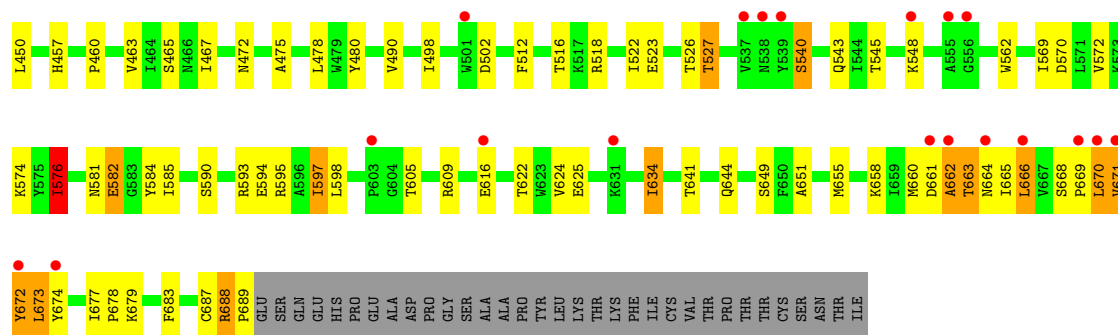
Chain	Residue	Modelled	Actual	Comment	Reference
B	125	GLY	-	expression tag	UNP P40763
B	126	SER	-	expression tag	UNP P40763
A	125	GLY	-	expression tag	UNP P40763
A	126	SER	-	expression tag	UNP P40763

- 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		



• Molecule 2: Monobody



• Molecule 2: Monobody



4 Data and refinement statistics

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) 99.7 (49.78-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.99%)	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)	0.30 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.97	2/4380 (0.0%)	1.11	9/5915 (0.2%)
1	B	1.00	5/4399 (0.1%)	1.15	15/5936 (0.3%)
2	C	0.99	1/746 (0.1%)	1.22	5/1028 (0.5%)
2	D	1.03	2/746 (0.3%)	1.15	3/1028 (0.3%)
All	All	0.99	10/10271 (0.1%)	1.14	32/13907 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	667	VAL	N-CA	6.16	1.54	1.46
1	B	667	VAL	CA-CB	6.03	1.62	1.54
2	D	83	PHE	N-CA	5.84	1.54	1.46
1	B	676	ASP	CB-CG	5.83	1.66	1.52
2	C	83	PHE	N-CA	5.63	1.54	1.46
1	B	676	ASP	CA-CB	5.57	1.62	1.53
1	B	664	ASN	N-CA	5.55	1.52	1.45
1	A	258	ILE	CA-C	5.15	1.59	1.52
2	D	4	VAL	CA-CB	5.06	1.60	1.54
1	A	625	GLU	CA-C	5.06	1.59	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	VAL	CA-C-N	-9.90	109.29	119.99
2	C	4	VAL	C-N-CA	-9.90	109.29	119.99
1	A	409	LYS	N-CA-C	-9.70	95.99	109.95
1	B	677	ILE	CB-CA-C	-7.55	102.17	110.85
1	A	665	ILE	N-CA-C	7.15	117.75	106.88
1	B	628	ILE	CB-CA-C	-7.04	102.51	112.22
1	A	214	ARG	CG-CD-NE	7.01	127.41	112.00
1	B	660	MET	N-CA-C	6.75	120.82	109.76
1	A	390	ASN	N-CA-CB	-6.65	101.43	110.67
1	B	576	ILE	N-CA-C	6.64	123.15	109.34
1	B	390	ASN	N-CA-CB	-6.58	101.52	110.67
2	C	4	VAL	N-CA-CB	6.51	120.33	111.21
1	B	151	VAL	N-CA-CB	6.09	118.83	110.54
2	C	39	THR	N-CA-C	6.07	118.39	111.11
1	A	163	LYS	N-CA-C	-5.95	104.73	112.23
1	B	625	GLU	N-CA-C	-5.87	102.79	110.53
1	B	667	VAL	N-CA-C	-5.86	97.16	109.34
1	A	518	ARG	N-CA-C	5.82	120.67	112.93
2	D	5	PRO	CA-N-CD	-5.76	103.94	112.00
1	B	254	GLY	CA-C-N	5.75	126.30	120.38
1	B	254	GLY	C-N-CA	5.75	126.30	120.38
2	D	4	VAL	O-C-N	5.68	127.57	121.10
1	B	667	VAL	N-CA-CB	5.62	120.50	111.23
1	A	672	TYR	N-CA-C	5.46	117.99	108.76
1	A	576	ILE	N-CA-C	5.44	120.66	109.34
1	B	153	LYS	N-CA-CB	5.43	119.40	110.39
1	B	575	TYR	N-CA-C	-5.16	102.51	109.95
1	B	550	CYS	N-CA-C	-5.14	101.45	108.24
1	A	191	ASN	N-CA-C	5.12	117.08	109.25
2	D	4	VAL	CA-C-O	-5.08	113.14	119.95
2	C	2	SER	N-CA-C	5.04	119.13	112.89
1	B	255	PRO	N-CA-C	5.03	116.84	110.70

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 ⓘ

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	111	0
1	B	4318	0	4362	80	0
2	C	723	0	702	24	1
2	D	723	0	702	34	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	10064	0	10095	244	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 12.

All (244) 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
1:A:660:MET:HE2	1:A:663:THR:O	1.68	0.92
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:641:THR:HG22	1:A:644:GLN:OE1	1.80	0.79
1:A:679:LYS:HD3	1:A:679:LYS:C	2.08	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:140:LYS:NZ	1:B:238:GLU:OE1	2.23	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
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:679:LYS:C	1:A:679:LYS:CD	2.73	0.61
1:B:575:TYR:C	1:B:576:ILE:HG22	2.25	0.60
1:A:576:ILE:HD12	1:A:585:ILE:CD1	2.32	0.60
1:B:655:MET:HE3	1:B:679:LYS:CD	2.31	0.59
1:A:670:LEU:HD23	1:A:670:LEU:O	2.02	0.59
1:B:164:VAL:CG2	1:B:213:MET:HE1	2.33	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:B:597:ILE:HG12	1:B:674:TYR:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:164:VAL:HG21	1:B:213:MET:HE1	1.84	0.57
2:D:3:SER:OG	2:D:5:PRO:O	2.23	0.57
2:D:33:HIS:CD2	2:D:49:THR:HG22	2.39	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:545:THR:HG23	1:B:548:LYS:H	1.71	0.56
1:A:677:ILE:HG22	1:A:678:PRO: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: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:605:THR:HG22	1:A:672:TYR:HB2	1.89	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:661:ASP:C	1:A:662:ALA:O	2.49	0.53
1:A:240:LEU:HA	1:A:263:LEU:HD11	1.91	0.53
2:D:34:ILE:HD13	2:D:72:VAL:HG22	1.90	0.53
2:C:78:TYR:HB3	2:C:79:PRO:HD3	1.89	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:655:MET:HE3	1:A:683:PHE:O	2.09	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:D:4:VAL:HG22	2:D:84:PRO:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:TYR:CD2	2:C:79:PRO:N	2.79	0.51
1:A:651:ALA:O	1:A:655:MET:SD	2.68	0.51
1:A:263:LEU:O	1:A:263:LEU:HD23	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: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: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
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
2:C:76:VAL:HB	2:C:82:TYR:HB3	1.93	0.49
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:671:VAL:HG12	1:A:672:TYR:CD1	2.49	0.48
1:A:410:HIS:C	1:A:411:LEU:HD12	2.40	0.47
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
1:A:329:MET:HE1	1:A:340:LYS:HB3	1.95	0.47
1:A:660:MET:CE	1:A:664:ASN:HA	2.44	0.47
2:C:4:VAL:HB	2:C:84:PRO:CG	2.44	0.47
1:B:498:ILE:HD12	1:B:543:GLN:CD	2.40	0.47
1:B:498:ILE:HD12	1:B:543:GLN:NE2	2.29	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
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:660:MET:HE2	1:A:664:ASN:HA	1.97	0.46
1:A:658:LYS:HB3	1:A:666:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:VAL:CG1	2:D:74:ALA:HB2	2.46	0.46
1:B:554:MET:O	1:B:556:GLY:N	2.48	0.46
1:A:576:ILE:HD12	1:A:585:ILE:HD11	1.96	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:660:MET:HE1	1:B:663:THR:O	2.16	0.46
1:A:329:MET:HE2	1:A:343:VAL:CG1	2.46	0.46
1:B:657:TYR:O	1:B:668:SER:HA	2.16	0.46
2:D:18:LEU:CD2	2:D:91:TYR:CD2	2.99	0.45
2:C:1:VAL:HG13	2:C:6:THR:HG22	1.97	0.45
1:B:203:LEU:HD23	1:B:206:MET:HE2	1.98	0.45
1:A:594:GLU:CD	1:A:609:ARG:HH11	2.24	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
1:B:310:VAL:HG13	1:B:450:LEU:HD21	1.99	0.45
1:B:667:VAL:O	1:B:668:SER:C	2.60	0.45
2:D:78:TYR:CB	2:D:79:PRO:HD3	2.45	0.45
1:B:655:MET:HE3	1:B:679:LYS:HG2	1.99	0.45
1:A:185:MET:O	1:A:188:LEU:HB3	2.17	0.45
1:B:225:LEU:HD12	1:B:305:LEU:HD23	1.99	0.44
1:A:366:VAL:HG23	1:A:441:PHE:CD1	2.52	0.44
1:B:655:MET:HE3	1:B:679:LYS:HD2	1.98	0.44
2:D:4:VAL:CB	2:D:5:PRO:CD	2.92	0.44
2:D:18:LEU:CD2	2:D:91:TYR:HD2	2.30	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
1:A:329:MET:HE2	1:A:343:VAL:HG11	1.98	0.44
1:A:581:ASN:O	1:A:582:GLU:HG2	2.18	0.44
2:D:4:VAL:HB	2:D:5:PRO:CD	2.47	0.44
1:B:242:ASP:HB3	1:B:246:ARG:NH2	2.32	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
2:D:18:LEU:HD21	2:D:91:TYR:HD2	1.83	0.44
1:B:161:LYS:HB3	1:B:217:ILE:HD11	1.99	0.43
1:A:225:LEU:HD12	1:A:305:LEU:HD23	2.00	0.43
1:B:575:TYR:O	1:B:576:ILE:HG22	2.18	0.43
1:A:598:LEU:HD13	1:A:624:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:CZ	1:A:297:PRO:HG3	2.48	0.43
1:B:575:TYR:C	1:B:576:ILE:CG2	2.92	0.43
1:B:607:LEU:CD2	1:B:622:THR:HB	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: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:B:252:ILE:HB	1:B:478:LEU:HD23	2.01	0.43
1:A:202:GLN:O	1:A:206:MET:HG2	2.19	0.43
1:A:594:GLU:CD	1:A:609:ARG:NH1	2.77	0.43
1:B:218:VAL:HG11	1:B:301:HIS:HB2	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
2:C:39:THR:HG23	2:C:67:ASP:O	2.19	0.43
2:D:18:LEU:HD22	2:D:91:TYR:CD2	2.54	0.42
2:C:4:VAL:HG11	2:C:74:ALA:N	2.34	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
1:A:398:GLU:C	1:A:400:ASN:N	2.78	0.42
2:D:66:VAL:HG13	2:D:68:TYR:CE2	2.54	0.42
1:A:597:ILE:HG12	1:A:674:TYR:CE1	2.54	0.42
1:B:197:ARG:HA	2:C:33:HIS:CE1	2.55	0.42
1:A:258:ILE:O	1:A:259:CYS:C	2.62	0.42
1:A:356:PRO:C	1:A:358:LEU:H	2.28	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
1:A:211:ASP:CG	1:A:215:ARG:HH21	2.29	0.41
2:D:82:TYR:O	2:D:83:PHE:HB2	2.20	0.41
1:B:654:ILE:HG23	1:B:670:LEU:CD1	2.50	0.41
1:A:136:VAL:HG23	1:A:136:VAL:O	2.20	0.41
1:A:475:ALA:HB2	1:A:562:TRP:CD1	2.54	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:A:330:PRO:HD3	1:A:345:PHE:HA	2.02	0.41
1:A:356:PRO:C	1:A:358:LEU:N	2.78	0.41
1:A:570:ASP:O	1:A:574:LYS:HG3	2.20	0.41
2:D:19:LEU:HD13	2:D:58:THR:CG2	2.49	0.41
1:A:594:GLU:C	1:A:597:ILE:HG22	2.45	0.41
1:B:576:ILE:O	1:B:576:ILE:CG1	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD13	1:A:221:LEU:CD2	2.50	0.41
1:A:670:LEU:O	1:A:670:LEU:CD2	2.68	0.41
1:B:195:VAL:CG2	2:C:49:THR:HG21	2.51	0.41
1:A:688:ARG:O	1:A:689:PRO:C	2.61	0.41
2:C:82:TYR:O	2:C:83:PHE:HB2	2.21	0.41
1:B:522:ILE:HD12	1:B:522:ILE:H	1.86	0.41
1:B:554:MET:O	1:B:555:ALA:C	2.64	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: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:B:211:ASP:CG	1:B:215:ARG:HH21	2.30	0.40
1:A:162:MET:HA	1:A:165:VAL:HG12	2.02	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: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 [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	525/598 (88%)	492 (94%)	22 (4%)	11 (2%)	5	21
1	B	527/598 (88%)	498 (94%)	21 (4%)	8 (2%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	93/95 (98%)	81 (87%)	9 (10%)	3 (3%)	3	13
2	D	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
All	All	1238/1386 (89%)	1155 (93%)	61 (5%)	22 (2%)	6	25

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 ⓘ

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%)	453 (95%)	26 (5%)	20	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	482/536 (90%)	453 (94%)	29 (6%)	17	47
2	C	82/82 (100%)	73 (89%)	9 (11%)	6	20
2	D	82/82 (100%)	77 (94%)	5 (6%)	17	46
All	All	1125/1236 (91%)	1056 (94%)	69 (6%)	17	46

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	GLU
1	B	154	ARG
1	B	186	GLN
1	B	188	LEU
1	B	191	ASN
1	B	197	ARG
1	B	214	ARG
1	B	219	SER
1	B	263	LEU
1	B	357	GLU
1	B	361	GLN
1	B	363	LYS
1	B	379	ARG
1	B	386	ILE
1	B	387	LEU
1	B	392	LYS
1	B	430	LEU
1	B	465	SER
1	B	498	ILE
1	B	502	ASP
1	B	522	ILE
1	B	527	THR
1	B	586	MET
1	B	593	ARG
1	B	597	ILE
1	B	600	THR
1	B	613	SER
1	B	628	ILE
1	B	688	ARG
1	A	143	MET
1	A	154	ARG
1	A	200	MET
1	A	203	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	ILE
1	A	219	SER
1	A	307	GLU
1	A	329	MET
1	A	357	GLU
1	A	363	LYS
1	A	382	ARG
1	A	386	ILE
1	A	465	SER
1	A	467	ILE
1	A	502	ASP
1	A	527	THR
1	A	540	SER
1	A	545	THR
1	A	548	LYS
1	A	582	GLU
1	A	597	ILE
1	A	616	GLU
1	A	634	ILE
1	A	649	SER
1	A	666	LEU
1	A	668	SER
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	4	VAL
2	C	16	THR
2	C	21	SER
2	C	33	HIS
2	C	53	SER
2	C	55	SER
2	C	80	GLU
2	C	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	205	GLN
1	B	280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	332	HIS
1	B	344	GLN
1	B	410	HIS
1	A	160	GLN
1	A	192	ASN
1	A	279	GLN
1	A	361	GLN
1	A	401	ASN
1	A	416	GLN
1	A	457	HIS
1	A	466	ASN
1	A	643	GLN
2	D	46	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	533/598 (89%)	0.44	39 (7%) 21 17	50, 80, 131, 183	0
1	B	535/598 (89%)	0.37	45 (8%) 17 14	48, 75, 122, 169	0
2	C	95/95 (100%)	0.47	3 (3%) 50 41	60, 86, 118, 135	0
2	D	95/95 (100%)	0.48	4 (4%) 40 32	57, 82, 120, 134	0
All	All	1258/1386 (90%)	0.42	91 (7%) 21 17	48, 78, 128, 183	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	667	VAL	6.3
1	B	666	LEU	6.0
1	A	398	GLU	5.4
1	B	661	ASP	5.3
1	B	258	ILE	5.3
1	A	670	LEU	5.3
1	B	662	ALA	5.2
1	A	661	ASP	4.7
1	A	428	ALA	4.6
1	A	294	LYS	4.6
1	A	400	ASN	4.5
1	A	603	PRO	4.3
1	A	258	ILE	4.0
1	A	331	MET	3.9
1	B	136	VAL	3.9
1	B	294	LYS	3.8
1	B	631	LYS	3.7
1	B	555	ALA	3.7
1	A	188	LEU	3.6
1	A	556	GLY	3.5
1	A	136	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	666	LEU	3.4
1	B	431	ILE	3.4
2	C	4	VAL	3.4
1	A	664	ASN	3.3
1	A	430	LEU	3.3
1	A	397	GLU	3.2
1	B	537	VAL	3.2
1	A	257	ASN	3.1
1	A	183	GLY	3.0
1	B	185	MET	3.0
1	A	259	CYS	2.9
1	B	665	ILE	2.9
1	B	675	PRO	2.8
1	B	688	ARG	2.8
1	B	400	ASN	2.8
1	B	160	GLN	2.8
1	A	662	ALA	2.8
1	B	663	THR	2.8
1	B	556	GLY	2.8
1	B	399	SER	2.7
1	B	188	LEU	2.7
1	B	398	GLU	2.7
1	B	599	SER	2.7
1	A	555	ALA	2.6
2	C	7	LYS	2.6
1	A	431	ILE	2.6
1	A	669	PRO	2.6
1	B	601	LYS	2.6
1	B	538	ASN	2.6
1	B	501	TRP	2.6
1	B	331	MET	2.5
1	A	414	ARG	2.5
1	B	418	CYS	2.5
1	A	548	LYS	2.5
1	A	631	LYS	2.5
1	B	255	PRO	2.5
1	B	600	THR	2.5
1	A	192	ASN	2.5
1	B	163	LYS	2.4
1	B	457	HIS	2.4
1	B	183	GLY	2.4
1	A	537	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	616	GLU	2.4
1	A	501	TRP	2.4
1	A	191	ASN	2.3
1	B	380	GLY	2.3
1	A	197	ARG	2.3
1	B	676	ASP	2.3
1	B	419	GLY	2.3
1	B	191	ASN	2.3
1	B	379	ARG	2.3
1	B	664	ASN	2.3
1	A	539	TYR	2.3
2	D	-1	GLY	2.3
1	A	674	TYR	2.2
1	A	185	MET	2.2
1	B	523	GLU	2.2
2	D	41	GLY	2.2
1	A	401	ASN	2.2
1	B	602	PRO	2.2
1	B	592	GLU	2.2
1	A	671	VAL	2.1
1	B	539	TYR	2.1
1	A	538	ASN	2.1
1	B	430	LEU	2.1
2	D	78	TYR	2.1
2	C	78	TYR	2.1
1	A	672	TYR	2.0
1	B	179	LEU	2.0
2	D	23	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.