Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 05:44 PM EST

PDB ID	:	3TIX
Title	:	Crystal structure of the Chp1-Tas3 complex core
Authors	:	Schalch, T.; Joshua-Tor, L.
Deposited on	:	2011-08-22
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:

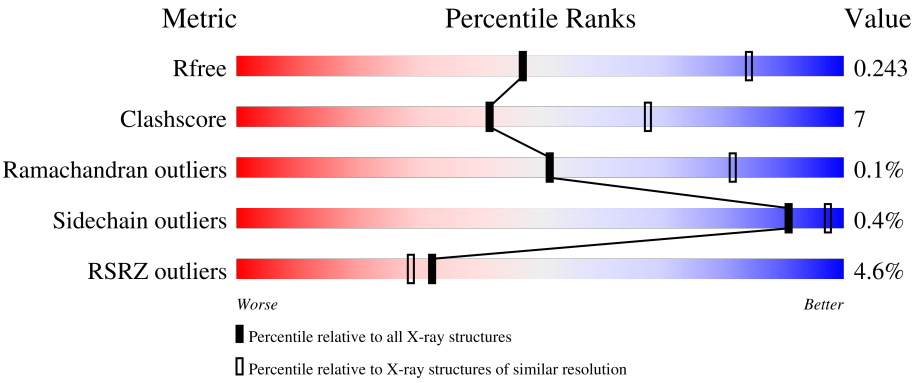
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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 <=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	207	3% 64% 10% 26%
1	C	207	2% 61% 10% 29%
2	B	458	3% 75% 17% 8%
2	D	458	6% 76% 17% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9309 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 Ubiquitin-like protein SMT3,RNA-induced transcriptional silencing complex protein tas3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1238	770	220	242	6			
1	C	147	Total	C	N	O	S	0	0	0
			1195	747	211	231	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-123	MET	-	initiating methionine	UNP Q12306
A	-122	SER	-	expression tag	UNP Q12306
A	-121	ALA	-	expression tag	UNP Q12306
A	-120	TRP	-	expression tag	UNP Q12306
A	-119	SER	-	expression tag	UNP Q12306
A	-118	HIS	-	expression tag	UNP Q12306
A	-117	PRO	-	expression tag	UNP Q12306
A	-116	GLN	-	expression tag	UNP Q12306
A	-115	PHE	-	expression tag	UNP Q12306
A	-114	GLU	-	expression tag	UNP Q12306
A	-113	LYS	-	expression tag	UNP Q12306
A	-112	GLY	-	expression tag	UNP Q12306
A	-111	GLY	-	expression tag	UNP Q12306
A	-110	GLY	-	expression tag	UNP Q12306
A	-109	SER	-	expression tag	UNP Q12306
A	-108	GLY	-	expression tag	UNP Q12306
A	-107	GLY	-	expression tag	UNP Q12306
A	-106	GLY	-	expression tag	UNP Q12306
A	-105	SER	-	expression tag	UNP Q12306
A	-104	GLY	-	expression tag	UNP Q12306
A	-103	GLY	-	expression tag	UNP Q12306
A	-102	SER	-	expression tag	UNP Q12306
A	-101	ALA	-	expression tag	UNP Q12306
A	-100	TRP	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-99	SER	-	expression tag	UNP Q12306
A	-98	HIS	-	expression tag	UNP Q12306
A	-97	PRO	-	expression tag	UNP Q12306
A	-96	GLN	-	expression tag	UNP Q12306
A	-95	PHE	-	expression tag	UNP Q12306
A	-94	GLU	-	expression tag	UNP Q12306
A	-93	LYS	-	expression tag	UNP Q12306
A	-92	THR	-	expression tag	UNP Q12306
A	-91	GLY	-	expression tag	UNP Q12306
A	-90	SER	-	expression tag	UNP Q12306
A	-89	LEU	-	expression tag	UNP Q12306
A	-88	GLN	-	expression tag	UNP Q12306
A	-26	THR	ARG	conflict	UNP Q12306
A	-19	GLU	ARG	conflict	UNP Q12306
C	-123	MET	-	initiating methionine	UNP Q12306
C	-122	SER	-	expression tag	UNP Q12306
C	-121	ALA	-	expression tag	UNP Q12306
C	-120	TRP	-	expression tag	UNP Q12306
C	-119	SER	-	expression tag	UNP Q12306
C	-118	HIS	-	expression tag	UNP Q12306
C	-117	PRO	-	expression tag	UNP Q12306
C	-116	GLN	-	expression tag	UNP Q12306
C	-115	PHE	-	expression tag	UNP Q12306
C	-114	GLU	-	expression tag	UNP Q12306
C	-113	LYS	-	expression tag	UNP Q12306
C	-112	GLY	-	expression tag	UNP Q12306
C	-111	GLY	-	expression tag	UNP Q12306
C	-110	GLY	-	expression tag	UNP Q12306
C	-109	SER	-	expression tag	UNP Q12306
C	-108	GLY	-	expression tag	UNP Q12306
C	-107	GLY	-	expression tag	UNP Q12306
C	-106	GLY	-	expression tag	UNP Q12306
C	-105	SER	-	expression tag	UNP Q12306
C	-104	GLY	-	expression tag	UNP Q12306
C	-103	GLY	-	expression tag	UNP Q12306
C	-102	SER	-	expression tag	UNP Q12306
C	-101	ALA	-	expression tag	UNP Q12306
C	-100	TRP	-	expression tag	UNP Q12306
C	-99	SER	-	expression tag	UNP Q12306
C	-98	HIS	-	expression tag	UNP Q12306
C	-97	PRO	-	expression tag	UNP Q12306
C	-96	GLN	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-95	PHE	-	expression tag	UNP Q12306
C	-94	GLU	-	expression tag	UNP Q12306
C	-93	LYS	-	expression tag	UNP Q12306
C	-92	THR	-	expression tag	UNP Q12306
C	-91	GLY	-	expression tag	UNP Q12306
C	-90	SER	-	expression tag	UNP Q12306
C	-89	LEU	-	expression tag	UNP Q12306
C	-88	GLN	-	expression tag	UNP Q12306
C	-26	THR	ARG	conflict	UNP Q12306
C	-19	GLU	ARG	conflict	UNP Q12306

- Molecule 2 is a protein called Chromo domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3411	2216	553	631	11			
2	D	424	Total	C	N	O	S	0	0	0
			3428	2229	555	633	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	503	MET	-	initiating methionine	UNP Q10103
D	503	MET	-	initiating methionine	UNP Q10103

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is water.

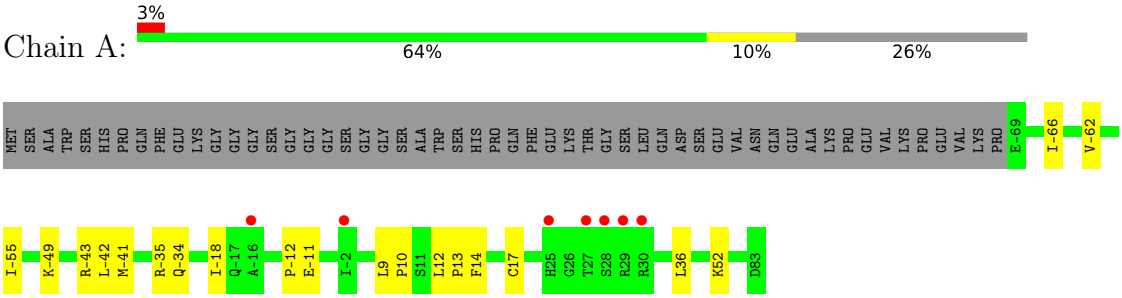
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	16	Total O 16 16	0	0
5	C	1	Total O 1 1	0	0
5	D	6	Total O 6 6	0	0

3 Residue-property plots

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.

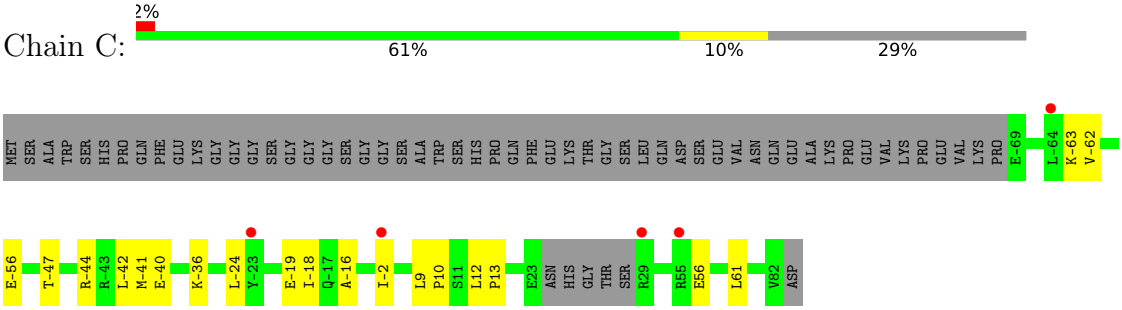
• Molecule 1: Ubiquitin-like protein SMT3,RNA-induced transcriptional silencing complex protein tas3

Chain A:



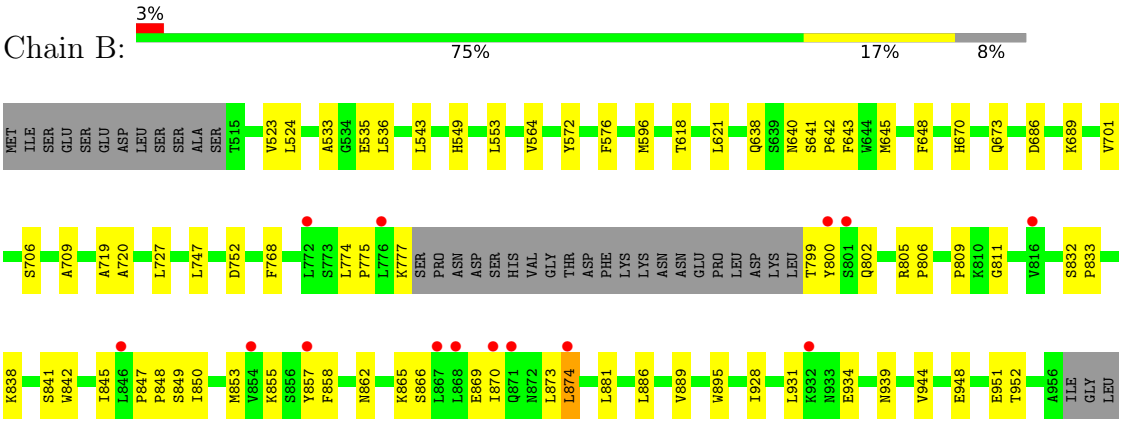
• Molecule 1: Ubiquitin-like protein SMT3,RNA-induced transcriptional silencing complex protein tas3

Chain C:



• Molecule 2: Chromo domain-containing protein 1

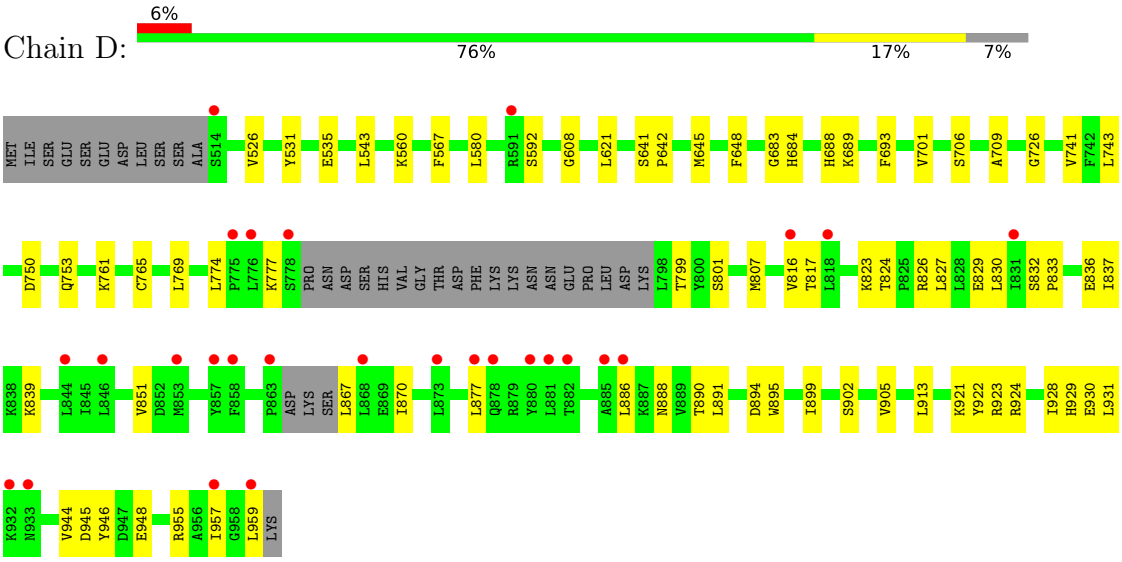
Chain B:



LYS

• Molecule 2: Chromo domain-containing protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.88Å 172.20Å 198.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.06 – 2.90 99.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.06-2.90) 99.8 (99.34-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.211 , 0.243 0.211 , 0.243	Depositor DCC
R_{free} test set	1997 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.020 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.031 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9309	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, K

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	0.21	0/1258	0.35	0/1691
1	C	0.21	0/1213	0.35	0/1628
2	B	0.22	0/3485	0.37	0/4723
2	D	0.21	0/3501	0.36	0/4744
All	All	0.22	0/9457	0.36	0/12786

There are no bond length outliers.

There are no bond angle outliers.

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	1238	0	1223	17	0
1	C	1195	0	1189	15	0
2	B	3411	0	3460	58	0
2	D	3428	0	3483	50	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	16	0	0	0	0
5	C	1	0	0	0	0
5	D	6	0	0	0	0
All	All	9309	0	9355	131	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 7.

All (131) 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)
2:D:765:CYS:O	2:D:923:ARG:NH2	2.20	0.74
2:B:832:SER:N	2:B:833:PRO:HD2	2.13	0.63
2:D:930:GLU:HG3	2:D:931:LEU:N	2.15	0.61
2:D:826:ARG:HG2	2:D:829:GLU:HB2	1.85	0.59
2:D:832:SER:N	2:D:833:PRO:HD2	2.18	0.59
1:C:-40:GLU:O	1:C:-36:LYS:HG2	2.02	0.59
2:D:837:ILE:HG21	2:D:957:ILE:CG2	2.33	0.58
1:C:9:LEU:N	1:C:10:PRO:HD2	2.19	0.58
2:B:800:TYR:CE1	2:B:806:PRO:HG3	2.40	0.57
2:B:849:SER:O	2:B:853:MET:HB2	2.05	0.57
2:B:701:VAL:HG12	2:B:747:LEU:CD1	2.35	0.57
2:B:774:LEU:HB3	2:B:777:LYS:HG2	1.87	0.56
1:C:-24:LEU:HD23	1:C:-19:GLU:HA	1.87	0.56
2:D:689:LYS:HG2	2:D:799:THR:HA	1.86	0.56
2:B:802:GLN:HA	2:D:895:TRP:HA	1.87	0.56
2:D:769:LEU:HG	2:D:807:MET:SD	2.47	0.55
2:B:928:ILE:HA	2:B:944:VAL:O	2.07	0.55
1:A:9:LEU:N	1:A:10:PRO:HD2	2.22	0.55
2:B:775:PRO:HB2	2:D:913:LEU:HD13	1.90	0.53
2:B:931:LEU:HB3	2:B:934:GLU:HB2	1.89	0.53
2:B:536:LEU:HD12	2:B:536:LEU:N	2.23	0.53
2:D:706:SER:HB2	2:D:709:ALA:HB3	1.91	0.53
2:D:641:SER:HB2	2:D:642:PRO:HD2	1.91	0.53
2:D:928:ILE:HA	2:D:944:VAL:O	2.08	0.53
2:B:638:GLN:NE2	2:B:640:ASN:OD1	2.42	0.53
1:C:-63:LYS:HD3	1:C:-56:GLU:HG3	1.91	0.52
2:B:524:LEU:HD12	2:B:533:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:951:GLU:HG3	2:B:952:THR:HG23	1.93	0.51
2:D:851:VAL:HA	2:D:877:LEU:HD23	1.93	0.50
2:D:839:LYS:HG2	2:D:888:ASN:OD1	2.11	0.50
2:B:564:VAL:HG21	2:B:621:LEU:HD12	1.93	0.50
2:D:688:HIS:CE1	2:D:693:PHE:CD2	2.99	0.50
2:D:535:GLU:HB3	2:D:592:SER:HB3	1.94	0.50
2:B:706:SER:HB2	2:B:709:ALA:HB3	1.94	0.50
2:B:886:LEU:HB2	2:B:889:VAL:HG23	1.94	0.49
1:C:-62:VAL:HG21	1:C:-42:LEU:HD21	1.95	0.49
1:C:12:LEU:N	1:C:13:PRO:HD2	2.27	0.49
2:D:560:LYS:HA	2:D:560:LYS:HE2	1.95	0.49
2:B:811:GLY:HA3	2:B:841:SER:O	2.13	0.49
2:D:816:VAL:HG12	2:D:817:THR:N	2.28	0.48
2:D:543:LEU:HD23	2:D:543:LEU:O	2.13	0.48
2:B:869:GLU:O	2:B:873:LEU:HG	2.13	0.48
2:B:870:ILE:O	2:B:874:LEU:HD23	2.13	0.48
2:B:689:LYS:HE2	2:B:799:THR:HA	1.96	0.48
1:A:-55:ILE:CD1	1:A:-35:ARG:HD3	2.44	0.48
1:A:52:LYS:HA	2:B:777:LYS:HD2	1.96	0.47
2:D:580:LEU:HB3	2:D:648:PHE:CD2	2.50	0.47
2:B:838:LYS:HB3	2:B:842:TRP:CD1	2.50	0.47
2:B:543:LEU:HD21	2:B:549:HIS:HB2	1.97	0.47
2:D:823:LYS:HD2	2:D:930:GLU:HB2	1.97	0.46
2:B:832:SER:N	2:B:833:PRO:CD	2.78	0.46
1:C:-63:LYS:HE2	1:C:-2:ILE:HG12	1.96	0.46
1:C:9:LEU:N	1:C:10:PRO:CD	2.79	0.46
1:C:-63:LYS:HD3	1:C:-56:GLU:CG	2.45	0.46
2:B:862:ASN:HB3	2:B:865:LYS:HG2	1.97	0.46
1:A:-43:ARG:HG3	1:A:-42:LEU:N	2.31	0.46
2:D:830:LEU:HD23	2:D:946:TYR:CZ	2.51	0.46
1:A:13:PRO:HA	1:A:36:LEU:HD13	1.97	0.45
2:D:959:LEU:C	2:D:959:LEU:HD13	2.36	0.45
2:B:621:LEU:HD23	2:B:645:MET:HG3	1.98	0.45
2:B:641:SER:HB2	2:B:642:PRO:CD	2.47	0.45
2:D:851:VAL:HA	2:D:877:LEU:CD2	2.46	0.45
1:A:-41:MET:HE1	1:A:-18:ILE:HB	1.97	0.45
1:A:-49:LYS:O	1:A:-11:GLU:HB2	2.16	0.45
2:B:862:ASN:HB3	2:B:865:LYS:CG	2.47	0.45
2:B:774:LEU:HB3	2:B:777:LYS:CG	2.46	0.44
2:B:895:TRP:HB3	2:D:801:SER:O	2.17	0.44
1:C:-41:MET:CE	1:C:-18:ILE:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:837:ILE:HG21	2:D:957:ILE:HG21	2.00	0.44
1:C:-42:LEU:C	1:C:-42:LEU:HD23	2.37	0.44
2:D:836:GLU:HB2	2:D:886:LEU:HD11	2.00	0.44
1:A:-62:VAL:HG21	1:A:-42:LEU:HD21	1.99	0.44
2:B:866:SER:O	2:B:870:ILE:HG12	2.17	0.44
2:D:944:VAL:HB	2:D:948:GLU:HB2	1.98	0.44
2:D:750:ASP:HB3	2:D:753:GLN:HG3	1.98	0.44
2:D:683:GLY:O	2:D:684:HIS:HB2	2.18	0.44
2:B:777:LYS:N	2:B:777:LYS:HD3	2.33	0.44
1:C:-44:ARG:HB2	1:C:-16:ALA:HB1	2.00	0.44
2:B:524:LEU:HB2	2:B:536:LEU:HD13	2.00	0.43
2:B:886:LEU:N	2:B:886:LEU:HD12	2.33	0.43
2:B:523:VAL:HG22	2:B:535:GLU:HG2	2.01	0.43
1:C:56:GLU:OE1	1:C:56:GLU:N	2.49	0.43
2:B:802:GLN:OE1	2:D:899:ILE:HG13	2.19	0.43
2:B:641:SER:CB	2:B:642:PRO:CD	2.96	0.43
2:B:862:ASN:CB	2:B:865:LYS:HG3	2.49	0.43
2:D:867:LEU:HA	2:D:870:ILE:HB	2.00	0.42
2:D:955:ARG:HD2	2:D:955:ARG:C	2.39	0.42
1:A:14:PHE:HB2	2:B:576:PHE:O	2.18	0.42
2:B:802:GLN:HG2	2:D:894:ASP:O	2.19	0.42
1:A:-66:ILE:HG23	1:A:-49:LYS:CE	2.49	0.42
2:B:944:VAL:HB	2:B:948:GLU:HB2	2.01	0.42
2:D:902:SER:HB3	2:D:905:VAL:HB	2.00	0.42
2:D:567:PHE:CZ	2:D:608:GLY:HA3	2.54	0.42
2:D:741:VAL:HG12	2:D:743:LEU:CD1	2.50	0.42
2:B:670:HIS:O	2:B:673:GLN:HG2	2.20	0.42
2:B:686:ASP:CG	2:B:689:LYS:HG2	2.40	0.42
2:D:823:LYS:CD	2:D:930:GLU:HB2	2.50	0.42
1:A:-34:GLN:N	1:A:-34:GLN:OE1	2.53	0.42
2:D:890:THR:HG22	2:D:891:LEU:N	2.35	0.42
2:D:923:ARG:HG2	2:D:924:ARG:HG2	2.02	0.42
1:C:61:LEU:HD12	2:D:774:LEU:HD11	2.02	0.41
1:A:12:LEU:N	1:A:13:PRO:HD2	2.35	0.41
2:B:618:THR:HB	2:B:648:PHE:HB2	2.01	0.41
2:B:799:THR:OG1	2:B:800:TYR:N	2.50	0.41
2:B:800:TYR:CZ	2:B:806:PRO:HG3	2.55	0.41
1:A:17:CYS:HB3	2:B:572:TYR:CD2	2.56	0.41
2:D:824:THR:O	2:D:827:LEU:HB2	2.20	0.41
2:D:929:HIS:O	2:D:945:ASP:HA	2.21	0.41
2:D:761:LYS:O	2:D:923:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-66:ILE:HG23	1:A:-49:LYS:HE3	2.02	0.41
1:A:9:LEU:N	1:A:10:PRO:CD	2.83	0.41
2:B:752:ASP:O	2:B:939:ASN:HB2	2.20	0.41
2:B:596:MET:HE3	2:B:643:PHE:CZ	2.56	0.41
2:B:805:ARG:HA	2:B:806:PRO:HD3	1.93	0.41
2:B:847:PRO:HA	2:B:848:PRO:HD3	1.97	0.41
2:B:850:ILE:HG21	2:B:881:LEU:HD11	2.03	0.41
2:B:845:ILE:HG23	2:B:845:ILE:O	2.21	0.41
2:B:719:ALA:O	2:B:720:ALA:HB3	2.22	0.40
2:B:855:LYS:HB2	2:B:874:LEU:HD11	2.03	0.40
2:D:526:VAL:HB	2:D:531:TYR:CZ	2.56	0.40
2:D:837:ILE:HG21	2:D:957:ILE:HG23	2.03	0.40
1:A:-66:ILE:CG2	1:A:-49:LYS:HE2	2.50	0.40
2:B:858:PHE:CD1	2:B:870:ILE:CD1	3.05	0.40
1:C:-63:LYS:C	1:C:-63:LYS:HD2	2.41	0.40
1:A:-66:ILE:HD11	1:A:-12:PRO:HB3	2.03	0.40
2:B:543:LEU:HB3	2:B:553:LEU:HD12	2.03	0.40
2:D:701:VAL:HG12	2:D:726:GLY:O	2.20	0.40
2:D:921:LYS:CD	2:D:922:TYR:CE2	3.05	0.40
2:D:621:LEU:HD23	2:D:645:MET:HG3	2.04	0.40
2:D:774:LEU:HD13	2:D:777:LYS:HE3	2.03	0.40
2:B:768:PHE:HE1	2:B:800:TYR:HE1	1.70	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	151/207 (73%)	149 (99%)	2 (1%)	0	100	100
1	C	143/207 (69%)	142 (99%)	1 (1%)	0	100	100
2	B	417/458 (91%)	407 (98%)	9 (2%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	418/458 (91%)	405 (97%)	13 (3%)	0	100 100
All	All	1129/1330 (85%)	1103 (98%)	25 (2%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	809	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	137/179 (76%)	137 (100%)	0	100 100
1	C	132/179 (74%)	131 (99%)	1 (1%)	81 94
2	B	389/423 (92%)	386 (99%)	3 (1%)	81 94
2	D	391/423 (92%)	391 (100%)	0	100 100
All	All	1049/1204 (87%)	1045 (100%)	4 (0%)	91 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	727	LEU
2	B	857	TYR
2	B	874	LEU
1	C	-47	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	933	ASN
2	D	550	GLN
2	D	878	GLN

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

Of 11 ligands modelled in this entry, 11 are 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	153/207 (73%)	0.52	7 (4%)	32	29	50, 98, 145, 166	0
1	C	147/207 (71%)	0.45	5 (3%)	45	40	49, 93, 144, 170	0
2	B	421/458 (91%)	0.48	14 (3%)	46	41	45, 72, 140, 184	0
2	D	424/458 (92%)	0.61	27 (6%)	19	15	51, 83, 161, 199	0
All	All	1145/1330 (86%)	0.53	53 (4%)	32	29	45, 81, 151, 199	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	868	LEU	5.3
2	D	873	LEU	5.0
2	D	880	TYR	4.3
2	B	846	LEU	4.3
1	A	27	THR	4.2
2	D	863	PRO	4.0
2	B	867	LEU	4.0
2	D	857	TYR	3.9
2	D	877	LEU	3.6
1	C	29	ARG	3.5
2	B	932	LYS	3.5
2	D	957	ILE	3.5
2	D	846	LEU	3.4
2	B	874	LEU	3.4
2	B	800	TYR	3.3
2	D	886	LEU	3.3
1	A	29	ARG	3.3
2	D	868	LEU	3.2
2	D	933	ASN	3.2
2	D	776	LEU	3.1
2	B	857	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	959	LEU	2.9
1	A	28	SER	2.9
2	B	801	SER	2.8
2	D	816	VAL	2.8
1	A	25	HIS	2.8
1	A	-16	ALA	2.7
2	D	514	SER	2.7
1	A	30	ARG	2.6
2	B	871	GLN	2.6
2	D	591	ARG	2.6
2	D	853	MET	2.6
2	D	858	PHE	2.5
1	C	-2	ILE	2.5
1	C	55	ARG	2.4
2	D	778	SER	2.4
2	B	870	ILE	2.4
2	D	885	ALA	2.3
2	B	854	VAL	2.3
2	D	844	LEU	2.3
2	B	772	LEU	2.3
2	D	882	THR	2.3
2	B	776	LEU	2.3
2	B	816	VAL	2.2
1	C	-23	TYR	2.2
1	C	-64	LEU	2.2
2	D	881	LEU	2.2
2	D	932	LYS	2.2
2	D	878	GLN	2.2
2	D	818	LEU	2.2
2	D	775	PRO	2.2
2	D	831	ILE	2.1
1	A	-2	ILE	2.1

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 monosaccharides 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
4	K	C	1001	1/1	0.61	0.27	109,109,109,109	0
4	K	D	1001	1/1	0.64	0.15	118,118,118,118	0
3	CL	C	1003	1/1	0.83	0.14	74,74,74,74	0
3	CL	C	1002	1/1	0.88	0.20	85,85,85,85	0
3	CL	D	1002	1/1	0.89	0.13	64,64,64,64	0
3	CL	A	1002	1/1	0.91	0.13	68,68,68,68	0
3	CL	A	1001	1/1	0.91	0.21	77,77,77,77	0
3	CL	D	1004	1/1	0.96	0.12	65,65,65,65	0
3	CL	B	1002	1/1	0.96	0.13	62,62,62,62	0
3	CL	A	1003	1/1	0.97	0.22	76,76,76,76	0
4	K	B	1001	1/1	0.97	0.11	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.