Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:08 PM GMT

PDB ID	:	4BL9
Title	:	Crystal structure of full-length human Suppressor of fused (SUFU) mutant lacking a regulatory subdomain (crystal form I)
Authors	:	Cherry, A.L.; Finta, C.; Karlstrom, M.; Toftgard, R.; Jovine, L.
Deposited on	:	2013-05-02
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

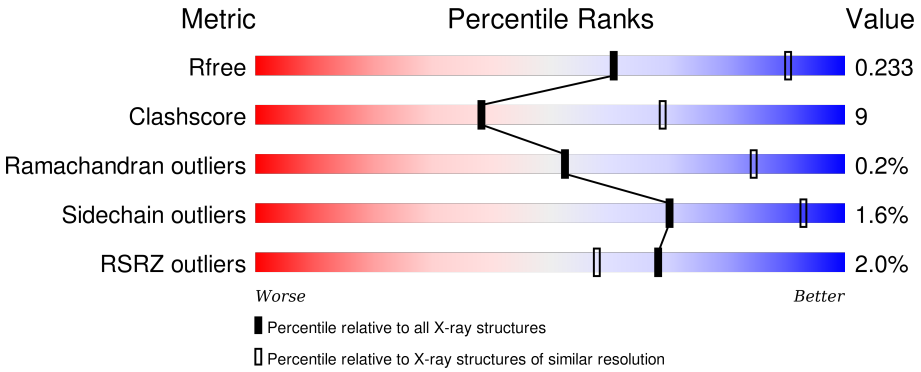
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	756	80% 15%
1	B	756	4% 76% 19%
1	C	756	80% 15%
1	D	756	2% 76% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22783 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 MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	0	0
			5651	3623	941	1069	18			
1	B	729	Total	C	N	O	S	0	0	0
			5705	3658	947	1082	18			
1	C	724	Total	C	N	O	S	0	0	0
			5667	3631	943	1075	18			
1	D	724	Total	C	N	O	S	0	0	0
			5668	3634	941	1075	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P0AEX9
A	3	THR	ILE	ENGINEERED MUTATION	UNP P0AEX9
A	360	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
A	363	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
A	364	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
A	368	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
A	369	ALA	-	LINKER	UNP P0AEX9
A	370	ALA	-	LINKER	UNP P0AEX9
A	371	ALA	-	LINKER	UNP P0AEX9
A	619	PRO	-	LINKER	UNP Q9UMX1
A	620	SER	-	LINKER	UNP Q9UMX1
A	621	ARG	-	LINKER	UNP Q9UMX1
A	622	GLY	-	LINKER	UNP Q9UMX1
A	623	GLU	-	LINKER	UNP Q9UMX1
A	624	ASP	-	LINKER	UNP Q9UMX1
A	625	PRO	-	LINKER	UNP Q9UMX1
A	749	VAL	-	EXPRESSION TAG	UNP Q9UMX1
A	750	GLU	-	EXPRESSION TAG	UNP Q9UMX1
A	751	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	752	HIS	-	EXPRESSION TAG	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	753	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	754	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	755	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	756	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	1	MET	-	EXPRESSION TAG	UNP P0AEX9
B	3	THR	ILE	ENGINEERED MUTATION	UNP P0AEX9
B	360	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
B	363	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
B	364	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
B	368	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
B	369	ALA	-	LINKER	UNP P0AEX9
B	370	ALA	-	LINKER	UNP P0AEX9
B	371	ALA	-	LINKER	UNP P0AEX9
B	619	PRO	-	LINKER	UNP Q9UMX1
B	620	SER	-	LINKER	UNP Q9UMX1
B	621	ARG	-	LINKER	UNP Q9UMX1
B	622	GLY	-	LINKER	UNP Q9UMX1
B	623	GLU	-	LINKER	UNP Q9UMX1
B	624	ASP	-	LINKER	UNP Q9UMX1
B	625	PRO	-	LINKER	UNP Q9UMX1
B	749	VAL	-	EXPRESSION TAG	UNP Q9UMX1
B	750	GLU	-	EXPRESSION TAG	UNP Q9UMX1
B	751	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	752	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	753	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	754	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	755	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	756	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	1	MET	-	EXPRESSION TAG	UNP P0AEX9
C	3	THR	ILE	ENGINEERED MUTATION	UNP P0AEX9
C	360	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
C	363	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
C	364	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
C	368	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
C	369	ALA	-	LINKER	UNP P0AEX9
C	370	ALA	-	LINKER	UNP P0AEX9
C	371	ALA	-	LINKER	UNP P0AEX9
C	619	PRO	-	LINKER	UNP Q9UMX1
C	620	SER	-	LINKER	UNP Q9UMX1
C	621	ARG	-	LINKER	UNP Q9UMX1
C	622	GLY	-	LINKER	UNP Q9UMX1
C	623	GLU	-	LINKER	UNP Q9UMX1

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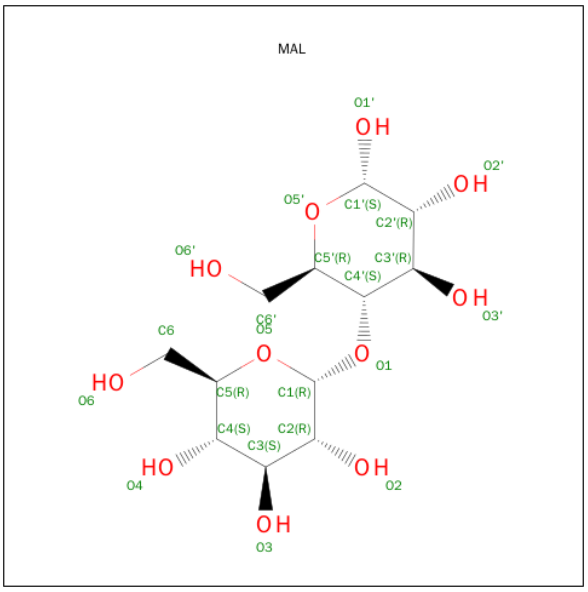
Chain	Residue	Modelled	Actual	Comment	Reference
C	624	ASP	-	LINKER	UNP Q9UMX1
C	625	PRO	-	LINKER	UNP Q9UMX1
C	749	VAL	-	EXPRESSION TAG	UNP Q9UMX1
C	750	GLU	-	EXPRESSION TAG	UNP Q9UMX1
C	751	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	752	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	753	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	754	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	755	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	756	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	1	MET	-	EXPRESSION TAG	UNP P0AEX9
D	3	THR	ILE	ENGINEERED MUTATION	UNP P0AEX9
D	360	ALA	GLU	ENGINEERED MUTATION	UNP P0AEX9
D	363	ALA	LYS	ENGINEERED MUTATION	UNP P0AEX9
D	364	ALA	ASP	ENGINEERED MUTATION	UNP P0AEX9
D	368	ASN	ARG	ENGINEERED MUTATION	UNP P0AEX9
D	369	ALA	-	LINKER	UNP P0AEX9
D	370	ALA	-	LINKER	UNP P0AEX9
D	371	ALA	-	LINKER	UNP P0AEX9
D	619	PRO	-	LINKER	UNP Q9UMX1
D	620	SER	-	LINKER	UNP Q9UMX1
D	621	ARG	-	LINKER	UNP Q9UMX1
D	622	GLY	-	LINKER	UNP Q9UMX1
D	623	GLU	-	LINKER	UNP Q9UMX1
D	624	ASP	-	LINKER	UNP Q9UMX1
D	625	PRO	-	LINKER	UNP Q9UMX1
D	749	VAL	-	EXPRESSION TAG	UNP Q9UMX1
D	750	GLU	-	EXPRESSION TAG	UNP Q9UMX1
D	751	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	752	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	753	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	754	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	755	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	756	HIS	-	EXPRESSION TAG	UNP Q9UMX1

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



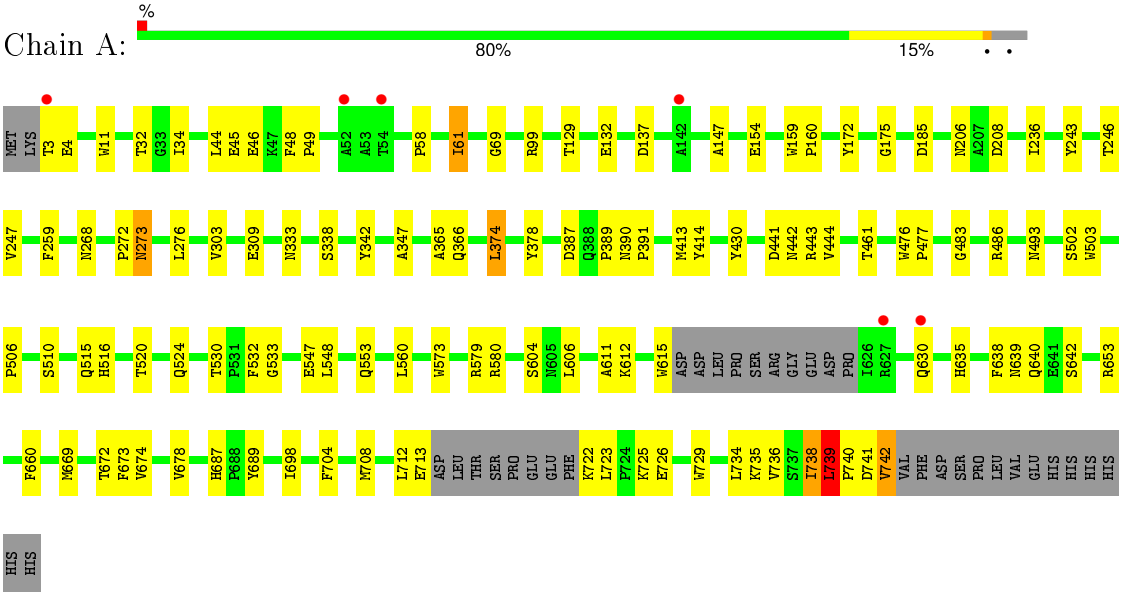
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	B	1	Total C O 23 12 11	0	0
2	C	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

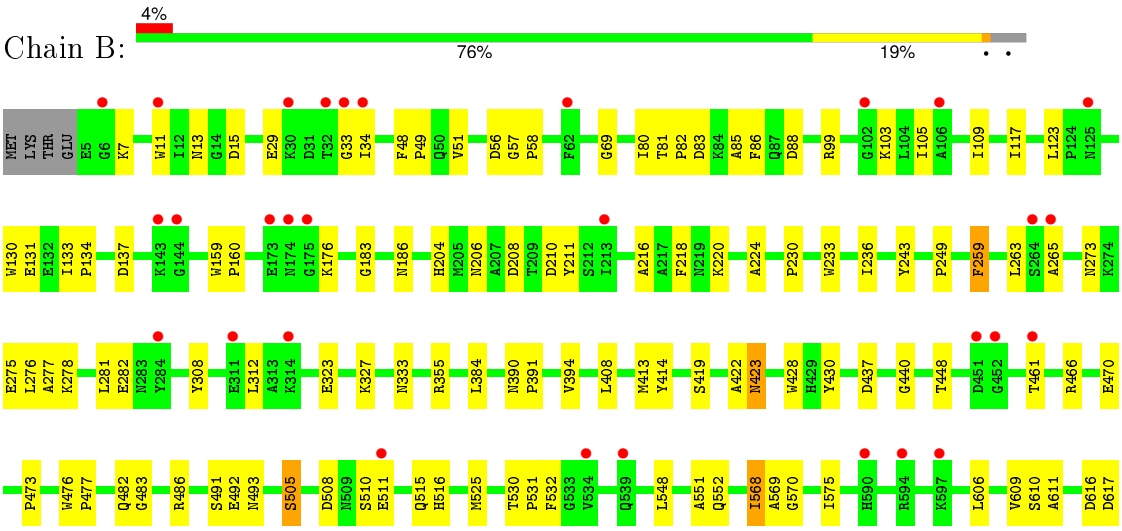
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

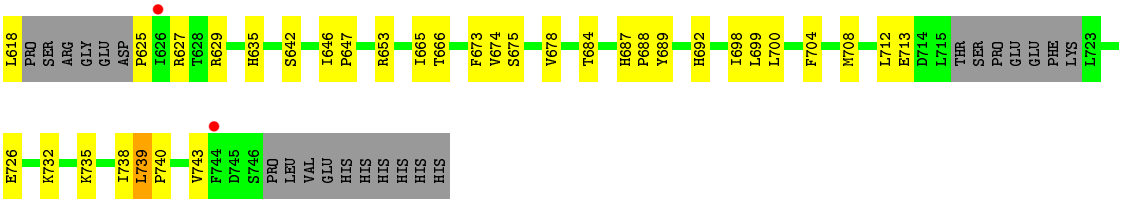
Chain A:



• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

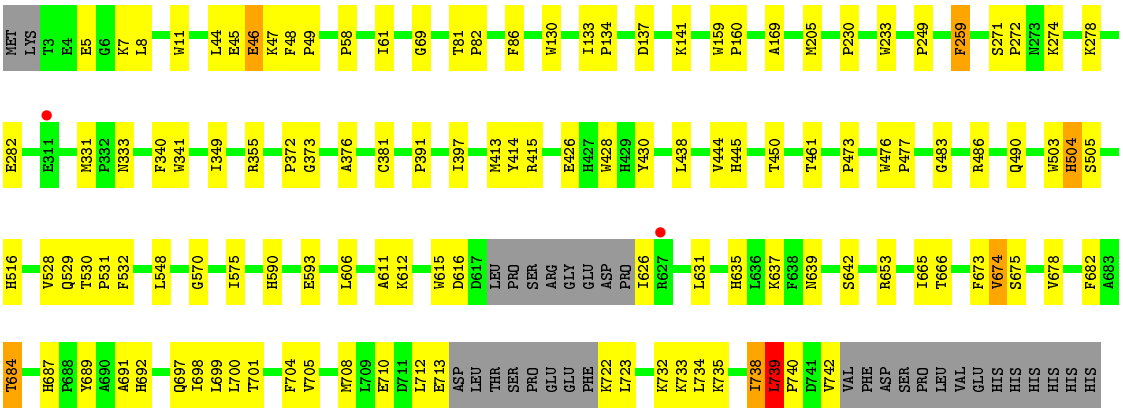
Chain B:





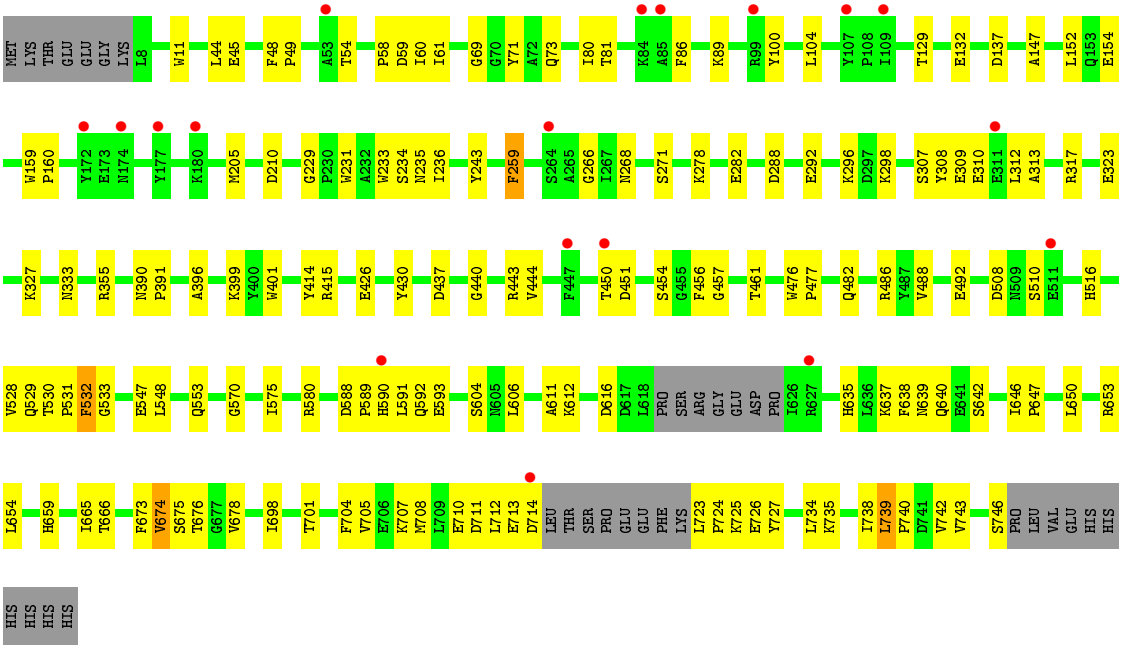
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain C:



• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.43Å 103.28Å 111.51Å 63.67° 81.13° 76.03°	Depositor
Resolution (Å)	29.48 – 2.80 29.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.48-2.80) 83.7 (29.48-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.200 , 0.234 0.197 , 0.233	Depositor DCC
R_{free} test set	2189 reflections (2.49%)	DCC
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 87952 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22783	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MAL

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	0.31	0/5801	0.46	0/7889
1	B	0.34	0/5857	0.46	0/7967
1	C	0.33	0/5817	0.45	0/7911
1	D	0.30	0/5819	0.44	0/7917
All	All	0.32	0/23294	0.45	0/31684

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	5651	0	5524	88	0
1	B	5705	0	5567	109	0
1	C	5667	0	5532	112	0
1	D	5668	0	5526	102	0
2	A	23	0	22	1	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
2	D	23	0	22	1	0
All	All	22783	0	22237	408	0

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

All (408) 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:C:635:HIS:NE2	1:C:735:LYS:HE2	1.65	1.11
1:C:635:HIS:CD2	1:C:637:LYS:HE2	2.06	0.90
1:B:505:SER:O	1:B:515:GLN:HA	1.78	0.82
1:A:4:GLU:O	1:A:273:ASN:ND2	2.11	0.82
1:C:635:HIS:CE1	1:C:735:LYS:HG2	2.15	0.82
1:C:635:HIS:HD2	1:C:637:LYS:HE2	1.44	0.81
1:A:45:GLU:O	1:A:49:PRO:CD	2.29	0.80
1:A:723:LEU:HD13	1:A:738:ILE:HG23	1.63	0.80
1:B:617:ASP:OD1	1:B:629:ARG:NH2	2.16	0.79
1:D:415:ARG:NH1	1:D:426:GLU:OE2	2.17	0.77
1:C:635:HIS:HD2	1:C:637:LYS:CE	1.98	0.77
1:B:29:GLU:O	1:B:33:GLY:CA	2.35	0.75
1:B:7:LYS:O	1:B:273:ASN:ND2	2.19	0.75
1:C:723:LEU:CD2	1:C:738:ILE:HG23	2.16	0.75
1:C:48:PHE:N	1:C:49:PRO:HD2	2.01	0.75
1:B:29:GLU:O	1:B:33:GLY:HA2	1.88	0.74
1:C:723:LEU:HD23	1:C:738:ILE:HG23	1.70	0.74
1:B:210:ASP:OD1	1:B:211:TYR:N	2.20	0.73
1:A:553:GLN:O	1:A:604:SER:HB2	1.89	0.72
1:A:45:GLU:O	1:A:49:PRO:HD3	1.87	0.72
1:C:635:HIS:NE2	1:C:735:LYS:CE	2.49	0.71
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.25	0.71
1:B:712:LEU:O	1:B:713:GLU:C	2.25	0.70
1:C:11:TRP:CD2	1:C:58:PRO:HG3	2.27	0.69
1:A:553:GLN:O	1:A:604:SER:CB	2.41	0.69
1:B:505:SER:O	1:B:515:GLN:CA	2.41	0.69
1:A:723:LEU:CD2	1:A:736:VAL:HG12	2.23	0.69
1:A:45:GLU:O	1:A:49:PRO:HD2	1.93	0.68
1:D:396:ALA:O	1:D:399:LYS:NZ	2.26	0.68
1:C:712:LEU:O	1:C:713:GLU:C	2.30	0.68
1:D:665:ILE:HG13	1:D:666:THR:HG23	1.75	0.68
1:B:29:GLU:O	1:B:33:GLY:N	2.25	0.68
1:D:235:ASN:OD1	1:D:298:LYS:NZ	2.26	0.68
1:B:611:ALA:HB1	1:B:642:SER:HB3	1.76	0.68
1:A:741:ASP:O	1:A:742:VAL:C	2.32	0.67
1:B:665:ILE:HG13	1:B:666:THR:HG23	1.76	0.66
1:B:123:LEU:HD23	1:B:224:ALA:HB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:TRP:CD2	1:B:58:PRO:HG2	2.30	0.65
1:D:391:PRO:HG3	1:D:414:TYR:CE1	2.33	0.64
1:C:48:PHE:CG	1:C:61:ILE:HD12	2.33	0.64
1:D:606:LEU:O	1:D:653:ARG:HD2	1.98	0.64
1:C:616:ASP:OD2	1:C:635:HIS:N	2.31	0.63
1:C:391:PRO:HG3	1:C:414:TYR:CZ	2.33	0.63
1:A:635:HIS:NE2	1:A:735:LYS:HG3	2.13	0.63
1:C:391:PRO:HG3	1:C:414:TYR:CE2	2.33	0.63
1:C:722:LYS:O	1:C:723:LEU:HD12	1.99	0.63
1:C:11:TRP:CD2	1:C:58:PRO:CG	2.82	0.63
1:B:625:PRO:O	1:B:627:ARG:HG3	2.00	0.62
1:B:708:MET:SD	1:B:732:LYS:NZ	2.73	0.62
1:C:739:LEU:N	1:C:740:PRO:CD	2.63	0.62
1:A:612:LYS:HB2	1:A:639:ASN:HB2	1.81	0.62
1:D:154:GLU:OE1	2:D:900:MAL:O6	2.18	0.62
1:A:69:GLY:HA3	1:A:333:ASN:O	2.00	0.61
1:A:712:LEU:O	1:A:713:GLU:C	2.38	0.61
1:D:530:THR:HG22	1:D:533:GLY:O	2.01	0.61
1:A:630:GLN:OE1	1:A:687:HIS:ND1	2.34	0.61
1:A:611:ALA:HB1	1:A:642:SER:HB3	1.82	0.60
1:B:423:ASN:OD1	1:B:423:ASN:C	2.39	0.60
1:B:69:GLY:HA3	1:B:333:ASN:O	2.00	0.60
1:A:11:TRP:CE3	1:A:58:PRO:HG3	2.37	0.59
1:D:547:GLU:OE2	1:D:580:ARG:NH2	2.37	0.58
1:A:524:GLN:NE2	1:A:573:TRP:CH2	2.71	0.58
1:A:723:LEU:CD1	1:A:738:ILE:HG23	2.34	0.58
1:D:159:TRP:N	1:D:160:PRO:CD	2.67	0.57
1:C:635:HIS:HA	1:C:733:LYS:O	2.04	0.57
1:C:159:TRP:N	1:C:160:PRO:CD	2.67	0.57
1:B:273:ASN:HB3	1:B:276:LEU:HD12	1.85	0.57
1:A:635:HIS:CE1	1:A:735:LYS:HD2	2.40	0.57
1:D:11:TRP:CG	1:D:58:PRO:HG3	2.40	0.57
1:A:185:ASP:HB2	1:A:366:GLN:HB2	1.85	0.57
1:A:443:ARG:HG3	1:A:444:VAL:HG23	1.87	0.57
1:B:355:ARG:NH1	1:B:390:ASN:OD1	2.37	0.56
1:C:11:TRP:CE2	1:C:58:PRO:HG3	2.39	0.56
1:C:530:THR:HG23	1:C:531:PRO:HD2	1.88	0.56
1:C:606:LEU:O	1:C:653:ARG:HD2	2.06	0.56
1:A:725:LYS:HB2	1:A:736:VAL:HB	1.87	0.56
1:B:323:GLU:O	1:B:327:LYS:HG3	2.05	0.56
1:C:710:GLU:O	1:C:713:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ALA:O	1:B:423:ASN:CB	2.54	0.56
1:B:422:ALA:O	1:B:423:ASN:CG	2.44	0.56
1:B:430:TYR:CZ	1:B:477:PRO:HG2	2.41	0.56
1:C:48:PHE:N	1:C:49:PRO:CD	2.68	0.55
1:B:476:TRP:CG	1:B:477:PRO:HD3	2.41	0.55
1:D:674:VAL:HG13	1:D:678:VAL:HG21	1.89	0.55
1:B:11:TRP:CD2	1:B:58:PRO:CG	2.89	0.55
1:B:159:TRP:N	1:B:160:PRO:CD	2.69	0.55
1:A:638:PHE:CD2	1:A:734:LEU:HD11	2.41	0.55
1:B:277:ALA:O	1:B:278:LYS:C	2.43	0.55
1:C:69:GLY:HA3	1:C:333:ASN:O	2.07	0.55
1:D:60:ILE:HA	1:D:266:GLY:O	2.06	0.55
1:D:701:THR:O	1:D:705:VAL:HG23	2.07	0.55
1:D:743:VAL:O	1:D:743:VAL:HG12	2.07	0.55
1:B:692:HIS:CE1	1:C:397:ILE:HD13	2.42	0.55
1:C:732:LYS:HG2	1:C:733:LYS:N	2.23	0.54
1:A:129:THR:OG1	1:A:132:GLU:HG3	2.07	0.54
1:D:355:ARG:NH1	1:D:390:ASN:OD1	2.40	0.54
1:C:684:THR:O	1:C:687:HIS:C	2.45	0.54
1:A:530:THR:HB	1:A:533:GLY:O	2.07	0.54
1:C:635:HIS:CD2	1:C:637:LYS:CE	2.78	0.54
1:D:86:PHE:O	1:D:89:LYS:HB2	2.08	0.54
1:B:133:ILE:N	1:B:134:PRO:CD	2.70	0.54
1:C:503:TRP:O	1:C:505:SER:N	2.41	0.54
1:C:612:LYS:HB2	1:C:639:ASN:HB2	1.88	0.54
1:C:476:TRP:CG	1:C:477:PRO:HD3	2.43	0.54
1:A:154:GLU:OE1	2:A:900:MAL:O6	2.22	0.54
1:C:391:PRO:CG	1:C:414:TYR:CZ	2.90	0.54
1:C:516:HIS:ND1	1:C:548:LEU:HD22	2.23	0.54
1:A:506:PRO:HG2	1:A:510:SER:O	2.08	0.54
1:C:415:ARG:NH1	1:C:426:GLU:OE2	2.40	0.54
1:A:673:PHE:CE2	1:A:698:ILE:HD11	2.43	0.54
1:D:73:GLN:OE1	1:D:100:TYR:OH	2.26	0.53
1:B:743:VAL:HG12	1:B:743:VAL:O	2.07	0.53
1:A:476:TRP:N	1:A:477:PRO:CD	2.71	0.53
1:B:684:THR:O	1:B:687:HIS:C	2.46	0.53
1:D:674:VAL:CG1	1:D:678:VAL:HG21	2.37	0.53
1:A:530:THR:HG22	1:A:532:PHE:H	1.74	0.53
1:D:739:LEU:HD12	1:D:739:LEU:C	2.28	0.53
1:B:265:ALA:CB	1:B:281:LEU:HD21	2.39	0.53
1:D:430:TYR:CZ	1:D:477:PRO:HG2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:PHE:CE2	1:B:708:MET:CE	2.91	0.52
1:A:476:TRP:CG	1:A:477:PRO:HD3	2.43	0.52
1:D:454:SER:O	1:D:457:GLY:N	2.41	0.52
1:A:159:TRP:N	1:A:160:PRO:CD	2.72	0.52
1:D:476:TRP:CG	1:D:477:PRO:HD3	2.44	0.52
1:D:476:TRP:N	1:D:477:PRO:CD	2.72	0.52
1:C:430:TYR:CZ	1:C:477:PRO:HG2	2.45	0.52
1:C:611:ALA:HB1	1:C:642:SER:HB3	1.91	0.52
1:C:615:TRP:CH2	1:C:691:ALA:CB	2.93	0.52
1:B:11:TRP:CE2	1:B:58:PRO:HG3	2.44	0.52
1:D:739:LEU:N	1:D:740:PRO:CD	2.73	0.52
1:C:673:PHE:CE2	1:C:698:ILE:HD11	2.45	0.52
1:C:46:GLU:O	1:C:49:PRO:HG2	2.11	0.51
1:D:516:HIS:ND1	1:D:548:LEU:HD22	2.24	0.51
1:C:81:THR:N	1:C:82:PRO:HD3	2.25	0.51
1:B:476:TRP:N	1:B:477:PRO:CD	2.73	0.51
1:B:85:ALA:O	1:B:88:ASP:HB2	2.09	0.51
1:B:391:PRO:CG	1:B:414:TYR:CE1	2.93	0.51
1:B:739:LEU:N	1:B:740:PRO:CD	2.73	0.51
1:B:508:ASP:OD1	1:B:510:SER:OG	2.23	0.51
1:C:11:TRP:CG	1:C:58:PRO:HG3	2.46	0.51
1:B:684:THR:O	1:B:687:HIS:O	2.28	0.51
1:B:616:ASP:OD2	1:B:635:HIS:N	2.42	0.51
1:D:707:LYS:O	1:D:710:GLU:HB2	2.11	0.51
1:B:510:SER:O	1:B:511:GLU:C	2.47	0.51
1:A:674:VAL:HG13	1:A:678:VAL:CG2	2.40	0.51
1:B:183:GLY:O	1:B:186:ASN:ND2	2.44	0.51
1:C:86:PHE:CE1	1:C:282:GLU:HG2	2.46	0.51
1:C:712:LEU:O	1:C:713:GLU:O	2.29	0.51
1:A:391:PRO:HG3	1:A:414:TYR:CE1	2.45	0.51
1:D:11:TRP:CG	1:D:58:PRO:CG	2.94	0.51
1:C:742:VAL:O	1:C:742:VAL:HG23	2.11	0.51
1:D:59:ASP:OD1	1:D:271:SER:OG	2.21	0.51
1:B:551:ALA:O	1:B:552:GLN:C	2.47	0.50
1:B:428:TRP:CE3	1:B:473:PRO:HB3	2.47	0.50
1:B:430:TYR:O	1:B:461:THR:HA	2.11	0.50
1:D:673:PHE:CE2	1:D:698:ILE:HD11	2.47	0.50
1:C:615:TRP:CE3	1:C:616:ASP:O	2.64	0.50
1:D:401:TRP:HB3	1:D:444:VAL:HG22	1.94	0.50
1:D:11:TRP:CD1	1:D:58:PRO:HG3	2.45	0.50
1:B:674:VAL:HG13	1:B:678:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:SER:O	1:A:653:ARG:NH1	2.45	0.50
1:B:708:MET:O	1:B:712:LEU:HD13	2.12	0.50
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.12	0.50
1:C:45:GLU:O	1:C:49:PRO:CD	2.59	0.50
1:A:606:LEU:O	1:A:653:ARG:HD2	2.12	0.50
1:B:674:VAL:HG13	1:B:678:VAL:HG22	1.93	0.50
1:B:394:VAL:HG23	1:B:413:MET:HE3	1.94	0.50
1:B:673:PHE:CE2	1:B:698:ILE:HD11	2.47	0.50
1:A:391:PRO:HG2	1:A:414:TYR:CZ	2.47	0.49
1:A:674:VAL:HG13	1:A:678:VAL:HG22	1.94	0.49
1:D:11:TRP:CD2	1:D:58:PRO:HG3	2.48	0.49
1:A:547:GLU:OE1	1:A:580:ARG:NH2	2.44	0.49
1:B:51:VAL:HB	1:B:56:ASP:HB3	1.93	0.49
1:A:46:GLU:C	1:A:49:PRO:HD2	2.33	0.49
1:D:443:ARG:HG3	1:D:444:VAL:HG23	1.94	0.49
1:D:323:GLU:O	1:D:327:LYS:HG3	2.12	0.49
1:D:612:LYS:HB2	1:D:639:ASN:HB2	1.94	0.49
1:D:570:GLY:HA2	1:D:575:ILE:O	2.11	0.49
1:C:45:GLU:HG2	1:C:46:GLU:N	2.26	0.49
1:A:172:TYR:CZ	1:A:175:GLY:HA2	2.47	0.49
1:C:635:HIS:NE2	1:C:735:LYS:HG2	2.28	0.49
1:B:394:VAL:HG23	1:B:413:MET:CE	2.41	0.49
1:D:723:LEU:HA	1:D:724:PRO:C	2.32	0.49
1:B:483:GLY:HA2	1:B:486:ARG:NH1	2.27	0.49
1:C:674:VAL:CG1	1:C:678:VAL:HG21	2.42	0.49
1:B:391:PRO:HG3	1:B:414:TYR:CE1	2.48	0.48
1:A:739:LEU:N	1:A:740:PRO:CD	2.76	0.48
1:A:46:GLU:O	1:A:49:PRO:HG2	2.12	0.48
1:D:450:THR:O	1:D:533:GLY:HA2	2.12	0.48
1:D:674:VAL:HG13	1:D:678:VAL:CG2	2.43	0.48
1:C:476:TRP:N	1:C:477:PRO:CD	2.76	0.48
1:B:11:TRP:CG	1:B:58:PRO:HG2	2.47	0.48
1:B:391:PRO:HG2	1:B:414:TYR:CE1	2.48	0.48
1:C:48:PHE:HB2	1:C:61:ILE:HD12	1.95	0.48
1:A:741:ASP:O	1:A:742:VAL:O	2.31	0.48
1:D:711:ASP:C	1:D:712:LEU:HD12	2.34	0.48
1:B:609:VAL:HG22	1:B:610:SER:N	2.28	0.48
1:D:80:ILE:HD11	1:D:104:LEU:HB3	1.96	0.48
1:A:430:TYR:O	1:A:461:THR:HA	2.14	0.48
1:B:137:ASP:OD2	1:B:204:HIS:ND1	2.47	0.48
1:D:137:ASP:HA	1:D:147:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ILE:HG22	1:C:355:ARG:NH2	2.29	0.48
1:D:236:ILE:HG22	1:D:243:TYR:CD2	2.49	0.48
1:C:137:ASP:O	1:C:141:LYS:HG2	2.14	0.48
1:D:11:TRP:CD2	1:D:58:PRO:CG	2.97	0.48
1:D:309:GLU:O	1:D:313:ALA:N	2.46	0.48
1:D:553:GLN:O	1:D:604:SER:OG	2.20	0.48
1:D:492:GLU:O	1:D:492:GLU:HG2	2.14	0.47
1:C:48:PHE:CB	1:C:61:ILE:HD12	2.44	0.47
1:D:665:ILE:CG1	1:D:666:THR:HG23	2.43	0.47
1:A:430:TYR:CZ	1:A:477:PRO:HG2	2.49	0.47
1:B:13:ASN:ND2	1:B:15:ASP:OD1	2.47	0.47
1:D:69:GLY:HA3	1:D:333:ASN:O	2.13	0.47
1:D:229:GLY:HA3	1:D:231:TRP:CH2	2.48	0.47
1:A:374:LEU:HD21	1:A:378:TYR:CE2	2.49	0.47
1:A:503:TRP:HB3	1:A:515:GLN:O	2.14	0.47
1:D:437:ASP:OD2	1:D:440:GLY:HA2	2.15	0.47
1:A:653:ARG:HD3	1:A:660:PHE:CD1	2.49	0.47
1:D:708:MET:O	1:D:712:LEU:HD13	2.15	0.47
1:D:588:ASP:O	1:D:591:LEU:HB2	2.14	0.47
1:A:45:GLU:HG2	1:A:46:GLU:N	2.30	0.47
1:C:503:TRP:O	1:C:504:HIS:C	2.51	0.47
1:B:606:LEU:O	1:B:653:ARG:HD2	2.15	0.47
1:D:456:PHE:CE2	1:D:488:VAL:HG12	2.50	0.47
1:C:723:LEU:HD22	1:C:738:ILE:HG23	1.94	0.47
1:D:430:TYR:O	1:D:461:THR:HA	2.15	0.47
1:C:11:TRP:HB3	1:C:44:LEU:HD11	1.96	0.46
1:B:81:THR:OG1	1:B:278:LYS:HE2	2.14	0.46
1:A:273:ASN:O	1:A:276:LEU:N	2.48	0.46
1:C:11:TRP:CG	1:C:58:PRO:CG	2.98	0.46
1:A:391:PRO:CG	1:A:414:TYR:CE1	2.99	0.46
1:D:391:PRO:HG2	1:D:414:TYR:CZ	2.49	0.46
1:A:630:GLN:OE1	1:A:687:HIS:CE1	2.68	0.46
1:D:80:ILE:CG1	1:D:104:LEU:HB3	2.46	0.46
1:A:726:GLU:OE1	1:A:735:LYS:HG2	2.15	0.46
1:B:80:ILE:O	1:B:82:PRO:HD3	2.16	0.46
1:C:530:THR:CG2	1:C:531:PRO:HD2	2.45	0.46
1:C:271:SER:O	1:C:274:LYS:NZ	2.49	0.46
1:A:48:PHE:N	1:A:49:PRO:HD2	2.30	0.46
1:D:391:PRO:CG	1:D:414:TYR:CZ	2.99	0.46
1:A:387:ASP:O	1:A:389:PRO:HD3	2.15	0.46
1:D:58:PRO:O	1:D:268:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:CD1	1:B:525:MET:HG2	2.46	0.46
1:A:44:LEU:HD12	1:A:44:LEU:C	2.36	0.46
1:D:589:PRO:O	1:D:592:GLN:HB3	2.15	0.46
1:C:734:LEU:O	1:C:734:LEU:HD12	2.15	0.46
1:C:616:ASP:O	1:C:616:ASP:OD1	2.33	0.46
1:A:653:ARG:HH11	1:A:653:ARG:HG2	1.80	0.46
1:B:278:LYS:O	1:B:282:GLU:HG3	2.16	0.46
1:D:637:LYS:HE2	1:D:735:LYS:HD2	1.97	0.46
1:A:516:HIS:ND1	1:A:548:LEU:HD22	2.31	0.46
1:A:547:GLU:OE2	1:A:580:ARG:NH2	2.49	0.45
1:C:665:ILE:HG13	1:C:666:THR:N	2.30	0.45
1:C:373:GLY:HA3	1:C:438:LEU:O	2.15	0.45
1:B:570:GLY:HA2	1:B:575:ILE:O	2.16	0.45
1:C:413:MET:HG2	1:C:430:TYR:CD2	2.51	0.45
1:A:3:THR:OG1	1:A:272:PRO:CD	2.65	0.45
1:D:482:GLN:O	1:D:486:ARG:HG3	2.16	0.45
1:B:308:TYR:CE2	1:B:312:LEU:HD11	2.51	0.45
1:C:45:GLU:O	1:C:49:PRO:HD2	2.17	0.45
1:B:532:PHE:N	1:B:532:PHE:CD1	2.83	0.45
1:A:704:PHE:CE2	1:A:708:MET:CE	2.99	0.45
1:A:137:ASP:HA	1:A:147:ALA:HB2	1.99	0.45
1:C:372:PRO:HB2	1:C:531:PRO:HD2	1.98	0.45
1:C:376:ALA:HB1	1:C:528:VAL:HG11	1.98	0.45
1:C:7:LYS:HG2	1:C:8:LEU:N	2.31	0.45
1:C:486:ARG:O	1:C:490:GLN:HG2	2.17	0.45
1:D:308:TYR:CE2	1:D:312:LEU:CD1	3.00	0.44
1:A:32:THR:HG22	1:A:34:ILE:HD13	1.99	0.44
1:A:615:TRP:CD1	1:A:669:MET:HE2	2.52	0.44
1:D:532:PHE:CD1	1:D:532:PHE:N	2.80	0.44
1:A:246:THR:OG1	1:A:247:VAL:N	2.50	0.44
1:D:234:SER:CB	1:D:298:LYS:HD3	2.47	0.44
1:C:428:TRP:CE3	1:C:473:PRO:HB3	2.52	0.44
1:C:5:GLU:HG3	1:C:272:PRO:HB2	1.99	0.44
1:C:11:TRP:CE3	1:C:44:LEU:CD1	3.00	0.44
1:B:265:ALA:HB3	1:B:281:LEU:CD2	2.47	0.44
1:C:704:PHE:CZ	1:C:708:MET:HE2	2.53	0.44
1:D:45:GLU:O	1:D:71:TYR:OH	2.32	0.44
1:B:83:ASP:OD2	1:B:86:PHE:N	2.48	0.44
1:B:34:ILE:N	1:B:34:ILE:HD12	2.32	0.44
1:D:80:ILE:HG12	1:D:104:LEU:HB3	2.00	0.44
1:A:338:SER:O	1:A:342:TYR:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:HD12	1:D:44:LEU:C	2.38	0.44
1:A:635:HIS:NE2	1:A:735:LYS:CD	2.80	0.44
1:C:704:PHE:CE2	1:C:708:MET:CE	3.01	0.44
1:D:638:PHE:CD2	1:D:734:LEU:HD11	2.53	0.44
1:A:413:MET:HG2	1:A:430:TYR:CD2	2.53	0.44
1:B:29:GLU:HA	1:B:34:ILE:O	2.18	0.43
1:B:419:SER:HB3	1:B:422:ALA:HB3	1.99	0.43
1:C:722:LYS:C	1:C:723:LEU:HD12	2.37	0.43
1:B:692:HIS:CE1	1:C:397:ILE:CD1	3.02	0.43
1:C:590:HIS:O	1:C:593:GLU:HB2	2.18	0.43
1:A:660:PHE:O	1:A:672:THR:HA	2.18	0.43
1:D:726:GLU:OE1	1:D:735:LYS:HG2	2.18	0.43
1:C:483:GLY:HA2	1:C:486:ARG:NH1	2.33	0.43
1:D:725:LYS:HG3	1:D:727:TYR:CE1	2.54	0.43
1:A:206:ASN:OD1	1:A:208:ASP:HB2	2.18	0.43
1:B:391:PRO:HG2	1:B:414:TYR:CZ	2.53	0.43
1:C:259:PHE:CD1	1:C:331:MET:HG2	2.54	0.43
1:D:508:ASP:OD1	1:D:510:SER:OG	2.31	0.43
1:D:616:ASP:OD2	1:D:635:HIS:N	2.49	0.43
1:C:530:THR:O	1:C:532:PHE:N	2.52	0.43
1:B:159:TRP:NE1	1:B:259:PHE:CD2	2.87	0.43
1:D:739:LEU:HB2	1:D:742:VAL:CG2	2.48	0.43
1:B:206:ASN:ND2	1:B:208:ASP:OD2	2.52	0.43
1:C:430:TYR:O	1:C:461:THR:HA	2.18	0.43
1:B:408:LEU:HB2	1:B:482:GLN:NE2	2.34	0.43
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.54	0.43
1:B:568:ILE:HG13	1:B:569:ALA:N	2.34	0.43
1:C:278:LYS:O	1:C:282:GLU:HB2	2.19	0.43
1:D:528:VAL:HG12	1:D:529:GLN:N	2.33	0.43
1:B:275:GLU:O	1:B:276:LEU:C	2.51	0.43
1:B:516:HIS:ND1	1:B:548:LEU:HD22	2.34	0.43
1:D:611:ALA:HB1	1:D:642:SER:HB3	2.00	0.43
1:C:570:GLY:HA2	1:C:575:ILE:O	2.19	0.43
1:D:288:ASP:OD1	1:D:307:SER:OG	2.33	0.42
1:C:504:HIS:H	1:C:516:HIS:CE1	2.38	0.42
1:D:640:GLN:HB2	1:D:723:LEU:HD21	2.00	0.42
1:C:674:VAL:HG13	1:C:678:VAL:HG21	2.00	0.42
1:D:704:PHE:CE2	1:D:708:MET:CE	3.02	0.42
1:B:130:TRP:CD1	1:B:249:PRO:HB2	2.54	0.42
1:B:466:ARG:NH2	1:B:470:GLU:O	2.53	0.42
1:B:99:ARG:HA	1:B:103:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:ILE:HG22	1:C:692:HIS:CE1	2.55	0.42
1:B:726:GLU:HG2	1:B:735:LYS:HG2	2.01	0.42
1:B:704:PHE:CE2	1:B:708:MET:HE1	2.55	0.42
1:D:399:LYS:HD2	1:D:401:TRP:CH2	2.54	0.42
1:C:615:TRP:CH2	1:C:691:ALA:HB1	2.55	0.42
1:A:48:PHE:CG	1:A:61:ILE:HD13	2.55	0.42
1:A:723:LEU:HD13	1:A:738:ILE:CG2	2.43	0.42
1:A:58:PRO:O	1:A:268:ASN:HB2	2.19	0.42
1:D:450:THR:OG1	1:D:451:ASP:N	2.52	0.42
1:C:530:THR:C	1:C:532:PHE:N	2.72	0.42
1:B:117:ILE:HG22	1:B:218:PHE:CZ	2.55	0.42
1:B:674:VAL:O	1:B:699:LEU:HA	2.19	0.42
1:B:688:PRO:HB2	1:B:689:TYR:CD1	2.55	0.42
1:B:216:ALA:O	1:B:220:LYS:HB2	2.19	0.42
1:A:723:LEU:HD23	1:A:736:VAL:HG12	2.00	0.42
1:B:57:GLY:HA2	1:B:58:PRO:HD3	1.88	0.42
1:D:653:ARG:NE	1:D:659:HIS:O	2.45	0.42
1:D:675:SER:O	1:D:678:VAL:HG13	2.20	0.42
1:B:482:GLN:O	1:B:486:ARG:HG3	2.20	0.42
1:D:590:HIS:O	1:D:593:GLU:HB2	2.20	0.42
1:A:347:ALA:HB2	1:A:365:ALA:HB2	2.02	0.42
1:B:712:LEU:O	1:B:713:GLU:O	2.38	0.42
1:B:646:ILE:N	1:B:647:PRO:CD	2.83	0.42
1:C:530:THR:C	1:C:532:PHE:H	2.23	0.41
1:D:308:TYR:CE2	1:D:312:LEU:HD12	2.54	0.41
1:C:444:VAL:HG12	1:C:445:HIS:CD2	2.55	0.41
1:A:236:ILE:CG2	1:A:243:TYR:CD1	3.03	0.41
1:C:635:HIS:CE1	1:C:735:LYS:CG	2.97	0.41
1:A:723:LEU:CD2	1:A:736:VAL:CG1	2.95	0.41
1:C:739:LEU:H	1:C:740:PRO:CD	2.33	0.41
1:D:530:THR:OG1	1:D:531:PRO:HD2	2.20	0.41
1:B:131:GLU:O	1:B:134:PRO:HD2	2.20	0.41
1:B:265:ALA:HB3	1:B:281:LEU:HD21	2.02	0.41
1:B:236:ILE:HG22	1:B:243:TYR:CD1	2.54	0.41
1:C:701:THR:O	1:C:705:VAL:HG23	2.19	0.41
1:C:635:HIS:NE2	1:C:735:LYS:CD	2.83	0.41
1:B:617:ASP:O	1:B:618:LEU:HB3	2.20	0.41
1:D:456:PHE:CE2	1:D:488:VAL:CG1	3.03	0.41
1:B:437:ASP:OD1	1:B:440:GLY:N	2.54	0.41
1:D:233:TRP:CH2	1:D:317:ARG:HB3	2.55	0.41
1:C:631:LEU:O	1:C:689:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:LEU:HD23	1:D:654:LEU:HD12	2.02	0.41
1:C:675:SER:O	1:C:678:VAL:HG13	2.20	0.41
1:D:456:PHE:CD2	1:D:488:VAL:CG1	3.03	0.41
1:B:491:SER:O	1:B:492:GLU:CB	2.68	0.41
1:A:99:ARG:NH1	1:B:176:LYS:NZ	2.68	0.41
1:C:381:CYS:HB3	1:C:414:TYR:CZ	2.55	0.41
1:A:726:GLU:CD	1:A:735:LYS:HG2	2.41	0.41
1:A:303:VAL:HG23	1:A:309:GLU:HB2	2.01	0.41
1:B:530:THR:HG22	1:B:531:PRO:HD2	2.03	0.41
1:C:11:TRP:CD2	1:C:58:PRO:HG2	2.54	0.41
1:C:739:LEU:H	1:C:740:PRO:HD3	1.85	0.41
1:D:646:ILE:HB	1:D:647:PRO:HD3	2.03	0.41
1:A:708:MET:HG3	1:A:729:TRP:CZ2	2.55	0.41
1:D:278:LYS:O	1:D:282:GLU:HB2	2.21	0.41
1:D:292:GLU:O	1:D:296:LYS:HG3	2.21	0.41
1:C:682:PHE:CZ	1:C:697:GLN:HG3	2.56	0.41
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.55	0.41
1:A:722:LYS:HA	1:A:725:LYS:HE3	2.03	0.41
1:D:48:PHE:CG	1:D:61:ILE:HD12	2.55	0.41
1:B:109:ILE:HB	1:B:263:LEU:O	2.21	0.41
1:B:159:TRP:N	1:B:160:PRO:HD2	2.36	0.41
1:B:699:LEU:HD23	1:B:700:LEU:N	2.36	0.41
1:A:441:ASP:O	1:A:442:ASN:HB2	2.21	0.41
1:D:159:TRP:NE1	1:D:259:PHE:CD2	2.89	0.40
1:B:675:SER:O	1:B:678:VAL:HG13	2.22	0.40
1:C:372:PRO:HB2	1:C:530:THR:HG23	2.02	0.40
1:D:48:PHE:HB3	1:D:49:PRO:HD3	2.04	0.40
1:C:169:ALA:HB2	1:C:340:PHE:CZ	2.55	0.40
1:D:210:ASP:OD1	1:D:210:ASP:C	2.60	0.40
1:C:528:VAL:HG12	1:C:529:GLN:N	2.35	0.40
1:C:699:LEU:HD23	1:C:700:LEU:N	2.36	0.40
1:A:520:THR:HB	1:A:560:LEU:HD13	2.02	0.40
1:B:618:LEU:C	1:B:618:LEU:HD12	2.41	0.40
1:D:739:LEU:HB2	1:D:742:VAL:HG22	2.02	0.40
1:D:152:LEU:HD21	1:D:205:MET:HE1	2.04	0.40
1:A:483:GLY:HA2	1:A:486:ARG:NH1	2.36	0.40
1:C:341:TRP:CD1	2:C:900:MAL:H4	2.57	0.40
1:B:48:PHE:N	1:B:49:PRO:HD2	2.37	0.40
1:C:133:ILE:N	1:C:134:PRO:CD	2.84	0.40
1:D:159:TRP:CD1	1:D:259:PHE:CD2	3.10	0.40
1:C:450:THR:HG22	1:C:531:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:TYR:CD1	1:A:689:TYR:N	2.84	0.40
1:C:130:TRP:CD1	1:C:249:PRO:HB2	2.56	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	716/756 (95%)	702 (98%)	13 (2%)	1 (0%)	56	87
1	B	723/756 (96%)	700 (97%)	22 (3%)	1 (0%)	56	87
1	C	718/756 (95%)	700 (98%)	16 (2%)	2 (0%)	46	79
1	D	718/756 (95%)	698 (97%)	19 (3%)	1 (0%)	56	87
All	All	2875/3024 (95%)	2800 (97%)	70 (2%)	5 (0%)	52	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	504	HIS
1	D	739	LEU
1	A	739	LEU
1	B	739	LEU
1	C	739	LEU

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	596/629 (95%)	584 (98%)	12 (2%)	63 90
1	B	603/629 (96%)	595 (99%)	8 (1%)	76 94
1	C	598/629 (95%)	590 (99%)	8 (1%)	76 94
1	D	599/629 (95%)	588 (98%)	11 (2%)	66 91
All	All	2396/2516 (95%)	2357 (98%)	39 (2%)	70 93

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	259	PHE
1	A	273	ASN
1	A	374	LEU
1	A	390	ASN
1	A	493	ASN
1	A	502	SER
1	A	579	ARG
1	A	640	GLN
1	A	738	ILE
1	A	739	LEU
1	A	742	VAL
1	B	105	ILE
1	B	259	PHE
1	B	423	ASN
1	B	448	THR
1	B	493	ASN
1	B	505	SER
1	B	568	ILE
1	B	738	ILE
1	C	46	GLU
1	C	47	LYS
1	C	205	MET
1	C	259	PHE
1	C	674	VAL
1	C	684	THR
1	C	738	ILE
1	C	739	LEU
1	D	54	THR
1	D	81	THR
1	D	259	PHE

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Mol	Chain	Res	Type
1	D	310	GLU
1	D	532	PHE
1	D	674	VAL
1	D	676	THR
1	D	713	GLU
1	D	714	ASP
1	D	738	ILE
1	D	746	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAL	A	900	-	24,24,24	0.54	0	35,35,35	0.61	0
2	MAL	B	900	-	24,24,24	0.52	0	35,35,35	0.66	0
2	MAL	C	900	-	24,24,24	0.51	0	35,35,35	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAL	D	900	-	24,24,24	0.52	0	35,35,35	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAL	A	900	-	-	0/8/48/48	0/2/2/2
2	MAL	B	900	-	-	0/8/48/48	0/2/2/2
2	MAL	C	900	-	-	0/8/48/48	0/2/2/2
2	MAL	D	900	-	-	0/8/48/48	0/2/2/2

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	MAL	1	0
2	C	900	MAL	1	0
2	D	900	MAL	1	0

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, 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	722/756 (95%)	-0.35	6 (0%) 87 81	35, 56, 94, 140	0
1	B	729/756 (96%)	-0.04	32 (4%) 38 26	41, 80, 126, 168	0
1	C	724/756 (95%)	-0.41	2 (0%) 94 92	32, 52, 91, 134	0
1	D	724/756 (95%)	-0.04	18 (2%) 61 48	39, 76, 140, 187	0
All	All	2899/3024 (95%)	-0.21	58 (2%) 68 58	32, 66, 122, 187	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	GLY	4.3
1	D	264	SER	4.3
1	B	590	HIS	4.2
1	C	627	ARG	4.2
1	B	144	GLY	4.0
1	D	107	TYR	3.9
1	D	174	ASN	3.6
1	B	284	TYR	3.5
1	B	34	ILE	3.3
1	B	264	SER	3.3
1	D	84	LYS	3.2
1	B	452	GLY	3.0
1	D	172	TYR	2.9
1	D	627	ARG	2.9
1	D	85	ALA	2.9
1	A	3	THR	2.8
1	B	265	ALA	2.8
1	B	30	LYS	2.8
1	B	174	ASN	2.7
1	B	143	LYS	2.7
1	A	52	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	32	THR	2.6
1	A	142	ALA	2.5
1	B	62	PHE	2.5
1	B	6	GLY	2.5
1	D	590	HIS	2.5
1	B	175	GLY	2.5
1	B	125	ASN	2.4
1	B	594	ARG	2.4
1	D	99	ARG	2.4
1	B	511	GLU	2.4
1	B	173	GLU	2.4
1	B	11	TRP	2.3
1	B	213	ILE	2.3
1	A	54	THR	2.3
1	B	451	ASP	2.3
1	B	461	THR	2.3
1	B	106	ALA	2.3
1	D	714	ASP	2.2
1	B	102	GLY	2.2
1	B	597	LYS	2.2
1	D	511	GLU	2.2
1	D	447	PHE	2.2
1	B	314	LYS	2.2
1	D	177	TYR	2.2
1	B	311	GLU	2.1
1	A	630	GLN	2.1
1	B	539	GLN	2.1
1	A	627	ARG	2.1
1	B	744	PHE	2.1
1	C	311	GLU	2.1
1	B	534	VAL	2.1
1	D	180	LYS	2.0
1	B	626	ILE	2.0
1	D	53	ALA	2.0
1	D	311	GLU	2.0
1	D	109	ILE	2.0
1	D	450	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	MAL	A	900	23/23	0.96	0.27	1.91	28,44,54,65	0
2	MAL	D	900	23/23	0.94	0.30	1.18	62,78,89,91	0
2	MAL	C	900	23/23	0.96	0.25	1.10	30,42,53,62	0
2	MAL	B	900	23/23	0.94	0.23	0.37	55,64,85,89	0

6.5 Other polymers (i)

There are no such residues in this entry.