Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:08 PM GMT

PDB ID	:	4BLD
Title	:	Crystal structure of a human Suppressor of fused (SUFU)-GLI3p complex
Authors	:	Cherry, A.L.; Finta, C.; Karlstrom, M.; De Sanctis, D.; 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:

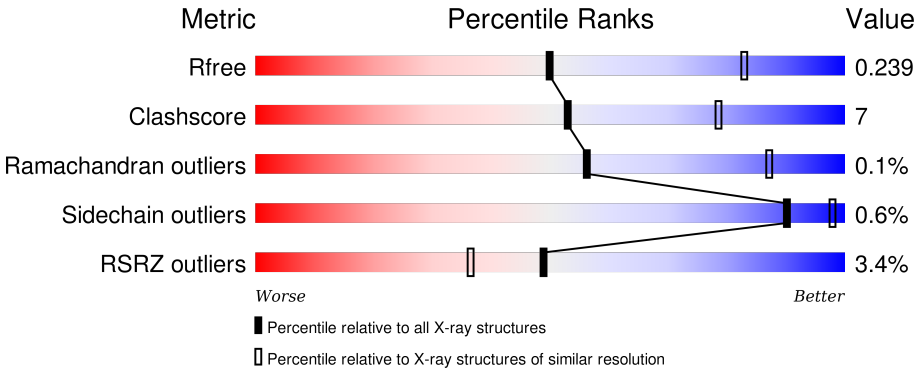
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	753	85% 12%
1	B	753	4% 81% 14% 5%
1	C	753	6% 82% 14%
1	D	753	2% 86% 11%
2	E	17	47% 53%

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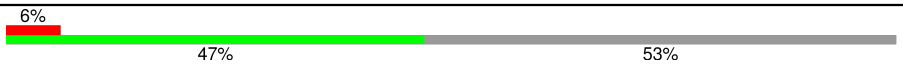
Mol	Chain	Length	Quality of chain
2	F	17	
2	G	17	
2	H	17	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23116 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	734	Total	C	N	O	S	0	0	0
			5757	3681	967	1090	19			
1	B	717	Total	C	N	O	S	0	0	0
			5621	3597	942	1064	18			
1	C	725	Total	C	N	O	S	0	0	0
			5687	3640	957	1072	18			
1	D	730	Total	C	N	O	S	0	0	0
			5727	3666	962	1081	18			

There are 120 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	401	ASP	TRP	ENGINEERED MUTATION	UNP Q9UMX1
A	402	SER	LEU	ENGINEERED MUTATION	UNP Q9UMX1
A	403	PHE	GLY	ENGINEERED MUTATION	UNP Q9UMX1
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	625	PRO	-	LINKER	UNP Q9UMX1
A	718	ALA	PRO	ENGINEERED MUTATION	UNP Q9UMX1
A	.	-	GLU	DELETION	UNP Q9UMX1
A	.	-	GLU	DELETION	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	PHE	DELETION	UNP Q9UMX1
A	719	ALA	LYS	ENGINEERED MUTATION	UNP Q9UMX1
A	746	VAL	-	EXPRESSION TAG	UNP Q9UMX1
A	747	GLU	-	EXPRESSION TAG	UNP Q9UMX1
A	748	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	749	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	750	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	751	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	752	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	753	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	401	ASP	TRP	ENGINEERED MUTATION	UNP Q9UMX1
B	402	SER	LEU	ENGINEERED MUTATION	UNP Q9UMX1
B	403	PHE	GLY	ENGINEERED MUTATION	UNP Q9UMX1
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	625	PRO	-	LINKER	UNP Q9UMX1
B	718	ALA	PRO	ENGINEERED MUTATION	UNP Q9UMX1
B	.	-	GLU	DELETION	UNP Q9UMX1
B	.	-	GLU	DELETION	UNP Q9UMX1
B	.	-	PHE	DELETION	UNP Q9UMX1
B	719	ALA	LYS	ENGINEERED MUTATION	UNP Q9UMX1
B	746	VAL	-	EXPRESSION TAG	UNP Q9UMX1
B	747	GLU	-	EXPRESSION TAG	UNP Q9UMX1
B	748	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	749	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	750	HIS	-	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
C	1	MET	-	EXPRESSION TAG	UNP P0AEX9
C	3	THR	ILE	ENGINEERED MUTATION	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
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	401	ASP	TRP	ENGINEERED MUTATION	UNP Q9UMX1
C	402	SER	LEU	ENGINEERED MUTATION	UNP Q9UMX1
C	403	PHE	GLY	ENGINEERED MUTATION	UNP Q9UMX1
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	625	PRO	-	LINKER	UNP Q9UMX1
C	718	ALA	PRO	ENGINEERED MUTATION	UNP Q9UMX1
C	.	-	GLU	DELETION	UNP Q9UMX1
C	.	-	GLU	DELETION	UNP Q9UMX1
C	.	-	PHE	DELETION	UNP Q9UMX1
C	719	ALA	LYS	ENGINEERED MUTATION	UNP Q9UMX1
C	746	VAL	-	EXPRESSION TAG	UNP Q9UMX1
C	747	GLU	-	EXPRESSION TAG	UNP Q9UMX1
C	748	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	749	HIS	-	EXPRESSION TAG	UNP Q9UMX1
C	750	HIS	-	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
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	401	ASP	TRP	ENGINEERED MUTATION	UNP Q9UMX1
D	402	SER	LEU	ENGINEERED MUTATION	UNP Q9UMX1
D	403	PHE	GLY	ENGINEERED MUTATION	UNP Q9UMX1
D	619	PRO	-	LINKER	UNP Q9UMX1
D	620	SER	-	LINKER	UNP Q9UMX1

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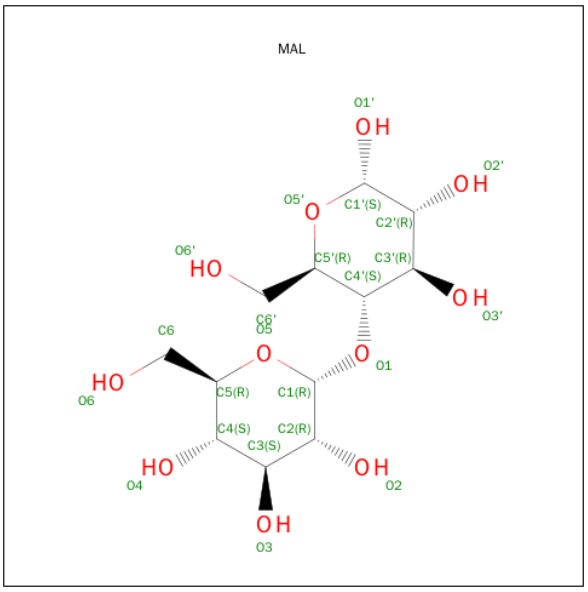
Chain	Residue	Modelled	Actual	Comment	Reference
D	621	ARG	-	LINKER	UNP Q9UMX1
D	622	GLY	-	LINKER	UNP Q9UMX1
D	625	PRO	-	LINKER	UNP Q9UMX1
D	718	ALA	PRO	ENGINEERED MUTATION	UNP Q9UMX1
D	.	-	GLU	DELETION	UNP Q9UMX1
D	.	-	GLU	DELETION	UNP Q9UMX1
D	.	-	PHE	DELETION	UNP Q9UMX1
D	719	ALA	LYS	ENGINEERED MUTATION	UNP Q9UMX1
D	746	VAL	-	EXPRESSION TAG	UNP Q9UMX1
D	747	GLU	-	EXPRESSION TAG	UNP Q9UMX1
D	748	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	749	HIS	-	EXPRESSION TAG	UNP Q9UMX1
D	750	HIS	-	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

- Molecule 2 is a protein called TRANSCRIPTIONAL ACTIVATOR GLI3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			57	35	10	12			
2	F	8	Total	C	N	O	0	0	0
			57	35	10	12			
2	G	8	Total	C	N	O	0	0	0
			57	35	10	12			
2	H	8	Total	C	N	O	0	0	0
			57	35	10	12			

- Molecule 3 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

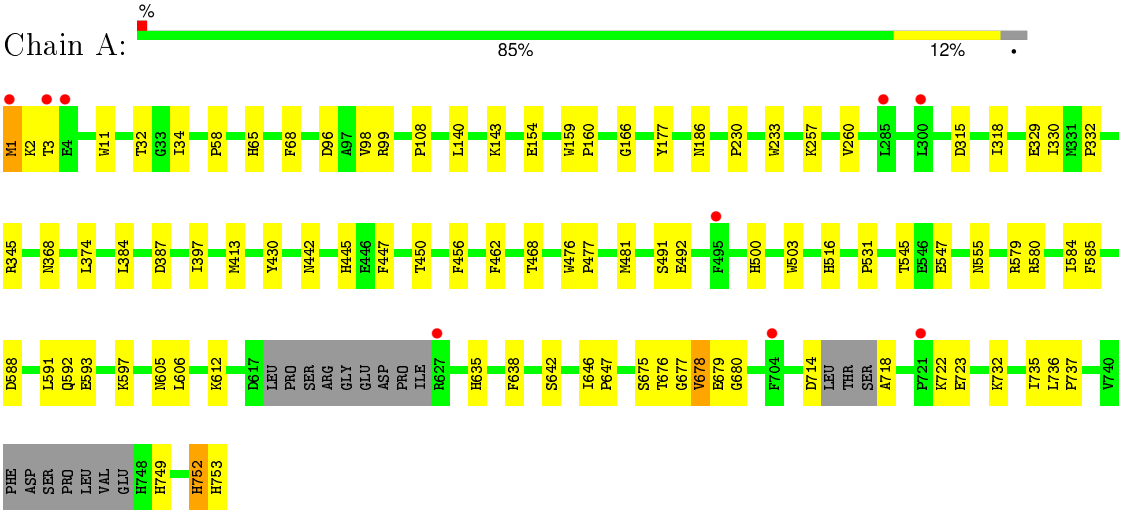
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

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.

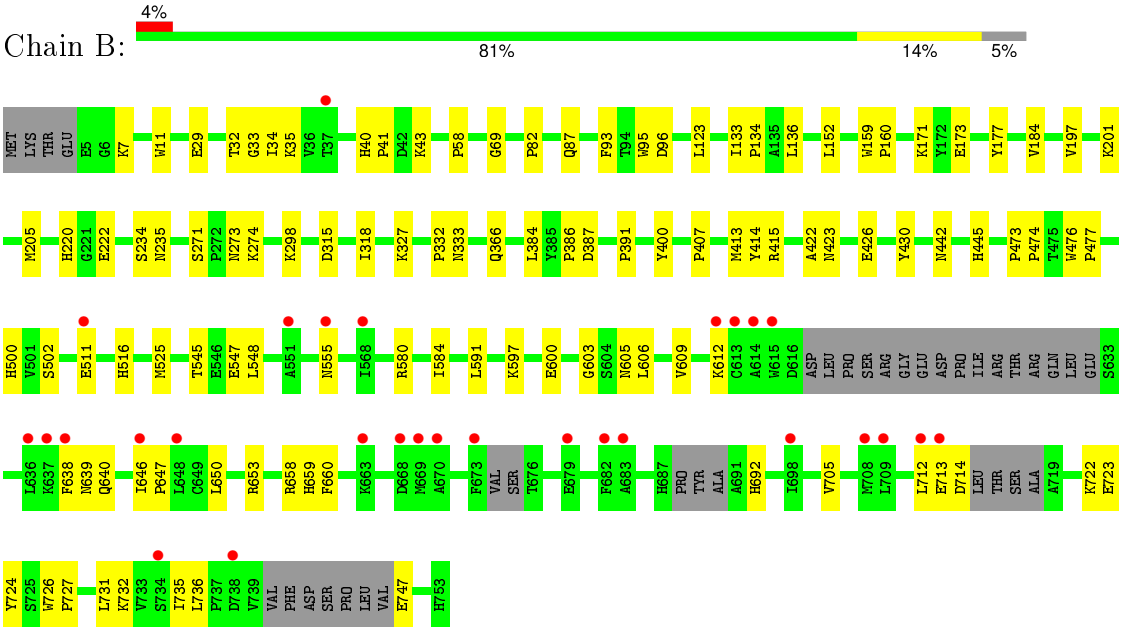
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain A:



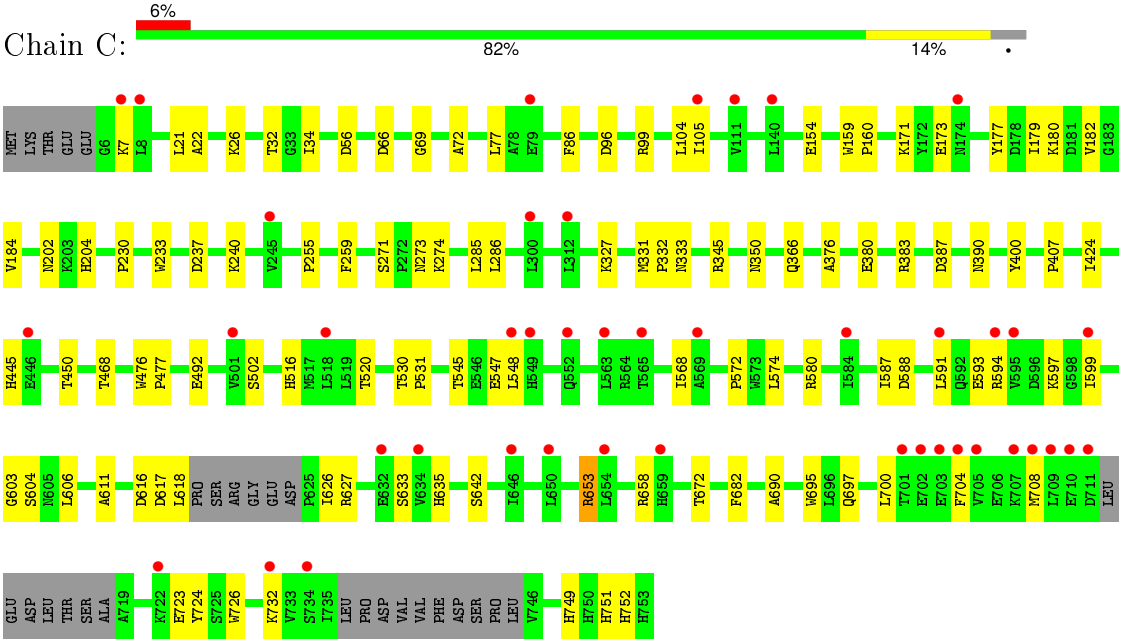
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain B:



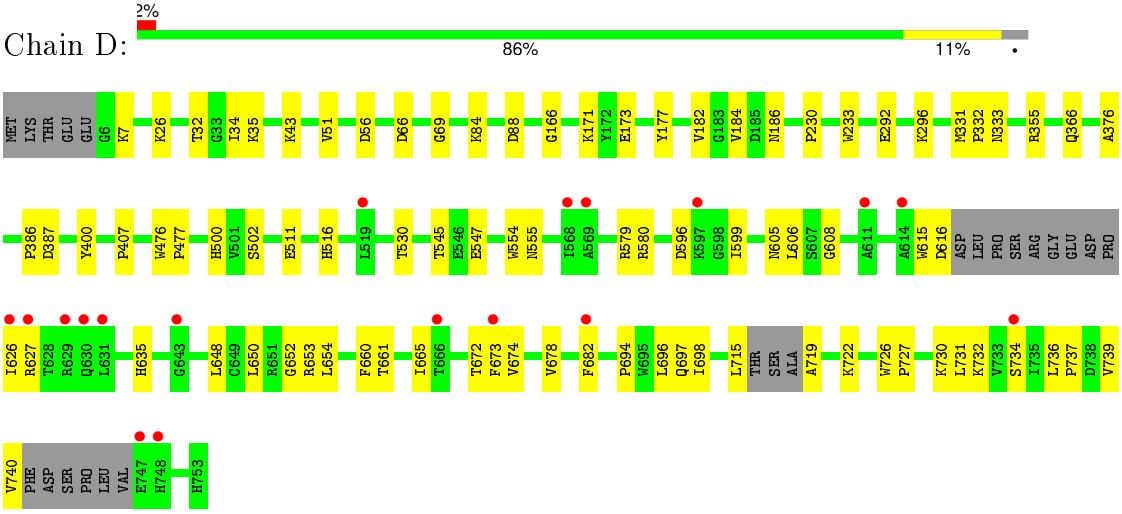
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain C:



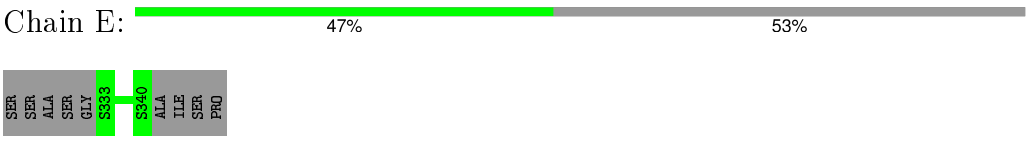
• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain D:



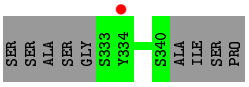
• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain E:



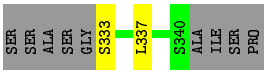
• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain F:



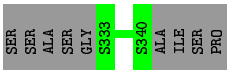
• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain G:



• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.61Å 136.55Å 116.74Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	19.94 – 2.80 46.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.94-2.80) 98.7 (46.36-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.234 0.205 , 0.239	Depositor DCC
R_{free} test set	1976 reflections (2.31%)	DCC
Wilson B-factor (Å^2)	75.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.4	EDS
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 85564 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23116	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% 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: ZN, 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	0.32	0/5913	0.57	0/8040
1	B	0.32	1/5773 (0.0%)	0.56	0/7847
1	C	0.33	0/5843	0.58	0/7945
1	D	0.31	0/5883	0.55	0/8001
2	E	0.21	0/58	0.48	0/77
2	F	0.19	0/58	0.30	0/77
2	G	0.22	0/58	0.42	0/77
2	H	0.23	0/58	0.43	0/77
All	All	0.32	1/23644 (0.0%)	0.56	0/32141

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	PRO	N-CD	5.36	1.55	1.47

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	5757	0	5587	75	0
1	B	5621	0	5442	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5687	0	5522	88	0
1	D	5727	0	5562	57	0
2	E	57	0	49	0	0
2	F	57	0	49	0	0
2	G	57	0	49	1	0
2	H	57	0	49	0	0
3	A	23	0	22	0	0
3	B	23	0	22	0	0
3	C	23	0	22	0	0
3	D	23	0	22	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	23116	0	22397	301	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 (301) 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:72:ALA:CB	1:C:105:ILE:HD13	1.45	1.44
1:A:585:PHE:CD1	1:A:591:LEU:HD11	1.72	1.25
1:C:72:ALA:HB1	1:C:105:ILE:HD13	1.19	1.19
1:D:51:VAL:HB	1:D:56:ASP:OD1	1.41	1.18
1:B:413:MET:HE3	1:B:430:TYR:CE2	1.77	1.18
1:C:72:ALA:CB	1:C:105:ILE:CD1	2.24	1.15
1:A:714:ASP:HB3	1:A:722:LYS:HZ1	1.13	1.13
1:B:712:LEU:HD12	1:B:713:GLU:N	1.65	1.12
1:C:72:ALA:HB2	1:C:105:ILE:HD13	1.21	1.09
1:C:77:LEU:HD13	1:C:105:ILE:HG22	1.30	1.09
1:C:72:ALA:HB1	1:C:105:ILE:CD1	1.84	1.06
1:B:413:MET:HE3	1:B:430:TYR:HE2	1.06	1.06
1:B:413:MET:CE	1:B:473:PRO:HB2	1.86	1.04
1:B:413:MET:CE	1:B:430:TYR:CE2	2.42	1.01
1:C:350:ASN:HD21	1:C:390:ASN:ND2	1.60	0.97
1:A:584:ILE:O	1:A:591:LEU:HD21	1.67	0.95
1:C:77:LEU:CD1	1:C:105:ILE:CG2	2.45	0.94
1:C:77:LEU:HD12	1:C:105:ILE:HG21	1.48	0.93
1:A:714:ASP:HB3	1:A:722:LYS:NZ	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASN:ND2	1:C:390:ASN:HD21	1.67	0.91
1:A:588:ASP:HB3	1:A:591:LEU:HD23	1.55	0.89
1:C:77:LEU:CD1	1:C:105:ILE:HG22	2.03	0.88
1:B:413:MET:HE2	1:B:473:PRO:HB2	1.54	0.88
1:B:413:MET:HE1	1:B:473:PRO:HB2	1.54	0.88
1:C:77:LEU:HD13	1:C:105:ILE:CG2	2.02	0.87
1:A:585:PHE:CD1	1:A:591:LEU:CD1	2.56	0.87
1:B:712:LEU:HD12	1:B:713:GLU:H	1.41	0.85
1:C:350:ASN:HD21	1:C:390:ASN:HD21	0.89	0.85
1:B:413:MET:CE	1:B:430:TYR:HE2	1.85	0.81
1:C:72:ALA:HB2	1:C:105:ILE:CD1	2.00	0.81
1:D:51:VAL:CB	1:D:56:ASP:OD1	2.27	0.80
1:A:585:PHE:HD1	1:A:591:LEU:HD11	1.43	0.79
1:A:585:PHE:CE1	1:A:591:LEU:HD11	2.17	0.79
1:C:77:LEU:CD1	1:C:105:ILE:HG21	2.12	0.79
1:B:413:MET:CE	1:B:474:PRO:O	2.33	0.77
1:A:584:ILE:O	1:A:591:LEU:CD2	2.32	0.77
1:B:413:MET:HE3	1:B:474:PRO:O	1.89	0.73
1:D:739:VAL:HG23	1:D:740:VAL:HG23	1.69	0.73
1:B:235:ASN:OD1	1:B:298:LYS:NZ	2.22	0.72
1:A:714:ASP:CB	1:A:722:LYS:HZ1	1.99	0.72
1:B:7:LYS:O	1:B:273:ASN:ND2	2.22	0.72
1:B:422:ALA:O	1:B:423:ASN:ND2	2.24	0.70
1:B:43:LYS:NZ	1:B:386:PRO:O	2.25	0.70
1:D:596:ASP:O	1:D:599:ILE:HG13	1.92	0.69
1:C:7:LYS:O	1:C:273:ASN:ND2	2.25	0.69
1:D:292:GLU:OE2	1:D:296:LYS:NZ	2.25	0.69
1:D:84:LYS:NZ	1:D:88:ASP:OD1	2.25	0.69
1:A:585:PHE:CE1	1:A:591:LEU:CD1	2.76	0.68
1:A:678:VAL:O	1:A:680:GLY:N	2.27	0.68
1:A:547:GLU:OE2	1:A:580:ARG:NH2	2.28	0.66
1:B:547:GLU:OE2	1:B:580:ARG:NH2	2.30	0.65
1:A:1:MET:HA	1:A:1:MET:HE2	1.80	0.64
1:B:712:LEU:CD1	1:B:713:GLU:N	2.54	0.64
1:C:182:VAL:O	1:C:366:GLN:NE2	2.29	0.64
1:D:555:ASN:HB3	1:D:605:ASN:HB2	1.79	0.63
1:B:639:ASN:OD1	1:B:640:GLN:N	2.29	0.63
1:A:723:GLU:OE1	1:A:732:LYS:NZ	2.32	0.62
1:D:736:LEU:O	1:D:739:VAL:HG22	1.99	0.62
1:D:648:LEU:O	1:D:652:GLY:N	2.32	0.62
1:B:234:SER:HB3	1:B:298:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG22	1:C:105:ILE:O	2.01	0.61
1:C:492:GLU:OE2	1:C:749:HIS:NE2	2.34	0.60
1:A:584:ILE:C	1:A:591:LEU:HD21	2.20	0.60
1:A:96:ASP:OD1	1:A:99:ARG:NH1	2.34	0.60
1:A:591:LEU:HD12	1:A:591:LEU:C	2.22	0.60
1:C:380:GLU:OE2	1:C:383:ARG:NH2	2.21	0.60
1:B:413:MET:HG2	1:B:430:TYR:CD2	2.36	0.60
1:C:154:GLU:OE1	1:C:345:ARG:NH1	2.34	0.60
1:A:555:ASN:HB3	1:A:605:ASN:HB2	1.83	0.60
1:B:413:MET:HE3	1:B:430:TYR:CZ	2.34	0.59
1:B:653:ARG:NE	1:B:659:HIS:O	2.33	0.59
1:D:7:LYS:HD3	1:D:35:LYS:HB3	1.83	0.59
1:C:547:GLU:OE2	1:C:580:ARG:NH2	2.35	0.59
1:D:674:VAL:CG1	1:D:678:VAL:HG21	2.32	0.59
1:C:350:ASN:ND2	1:C:390:ASN:ND2	2.37	0.59
1:C:72:ALA:HB2	1:C:105:ILE:HG21	1.84	0.58
1:B:413:MET:HE2	1:B:430:TYR:CE2	2.37	0.58
1:B:413:MET:HE1	1:B:474:PRO:O	2.02	0.58
1:B:712:LEU:CD1	1:B:713:GLU:H	2.16	0.58
1:A:492:GLU:OE2	1:A:749:HIS:CD2	2.57	0.58
1:B:82:PRO:HB2	1:B:87:GLN:HG3	1.85	0.58
1:A:468:THR:OG1	1:D:511:GLU:OE2	2.21	0.57
1:B:511:GLU:OE1	1:C:468:THR:OG1	2.22	0.57
1:A:154:GLU:OE1	1:A:345:ARG:NH1	2.37	0.57
1:B:502:SER:HA	1:B:516:HIS:HD2	1.68	0.57
1:C:271:SER:O	1:C:274:LYS:NZ	2.36	0.57
1:C:700:LEU:HD13	1:C:708:MET:HE1	1.87	0.56
1:C:568:ILE:HD11	1:C:587:ILE:HD13	1.87	0.56
1:B:413:MET:CE	1:B:430:TYR:CZ	2.89	0.55
1:B:234:SER:CB	1:B:298:LYS:HD3	2.35	0.55
1:C:682:PHE:CZ	1:C:697:GLN:HB2	2.41	0.55
1:C:77:LEU:CB	1:C:105:ILE:CG2	2.85	0.55
1:D:672:THR:HB	1:D:697:GLN:HG2	1.89	0.55
1:D:43:LYS:NZ	1:D:386:PRO:O	2.40	0.55
1:A:638:PHE:HB3	1:A:642:SER:OG	2.07	0.55
1:A:1:MET:HE1	1:A:2:LYS:H	1.71	0.55
1:A:585:PHE:CD1	1:A:592:GLN:OE1	2.59	0.54
1:A:585:PHE:HD1	1:A:591:LEU:CD1	2.11	0.54
1:D:608:GLY:HA3	1:D:661:THR:CG2	2.37	0.54
1:A:677:GLY:O	1:A:678:VAL:HG22	2.08	0.53
1:D:166:GLY:O	1:D:186:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:730:LYS:O	1:D:731:LEU:HD12	2.09	0.53
1:D:696:LEU:HD21	1:D:698:ILE:HG23	1.90	0.53
1:D:608:GLY:HA3	1:D:661:THR:HG22	1.91	0.53
1:B:603:GLY:HA3	1:B:658:ARG:HH22	1.74	0.53
1:D:547:GLU:OE2	1:D:580:ARG:NH2	2.42	0.52
1:D:696:LEU:CD2	1:D:698:ILE:HG23	2.40	0.52
1:D:182:VAL:O	1:D:366:GLN:NE2	2.34	0.52
1:B:32:THR:HG22	1:B:34:ILE:HD13	1.92	0.51
1:C:635:HIS:CE1	1:C:732:LYS:HG3	2.45	0.51
1:B:555:ASN:HB3	1:B:605:ASN:HB2	1.92	0.51
1:B:271:SER:O	1:B:274:LYS:NZ	2.28	0.51
1:C:682:PHE:CE1	1:C:690:ALA:HB3	2.46	0.51
1:C:626:ILE:HG22	1:C:627:ARG:HG3	1.93	0.51
1:C:502:SER:HA	1:C:516:HIS:HD2	1.76	0.51
1:C:611:ALA:HB1	1:C:642:SER:HB3	1.93	0.51
1:D:719:ALA:O	1:D:722:LYS:HE3	2.11	0.51
1:A:65:HIS:HA	1:A:68:PHE:CD2	2.46	0.50
1:B:234:SER:HB3	1:B:298:LYS:CD	2.41	0.50
1:C:255:PRO:CB	1:C:327:LYS:HD3	2.41	0.50
1:C:599:ILE:O	1:C:603:GLY:N	2.44	0.50
1:C:516:HIS:CD2	1:C:548:LEU:HD22	2.47	0.50
1:D:616:ASP:O	1:D:635:HIS:N	2.43	0.50
1:C:77:LEU:CB	1:C:105:ILE:HG23	2.42	0.49
1:B:184:VAL:HG23	1:B:366:GLN:HB2	1.94	0.49
1:B:650:LEU:HB3	1:B:705:VAL:HG13	1.93	0.49
1:C:672:THR:HB	1:C:697:GLN:HG2	1.93	0.49
1:B:724:TYR:HB3	1:B:726:TRP:CH2	2.48	0.49
1:D:500:HIS:CE1	1:D:606:LEU:HD21	2.47	0.49
1:D:653:ARG:HD3	1:D:660:PHE:HB2	1.94	0.49
1:A:723:GLU:OE1	1:A:732:LYS:HG2	2.12	0.49
1:C:516:HIS:CE1	1:C:545:THR:HG22	2.49	0.48
1:D:69:GLY:HA3	1:D:333:ASN:O	2.13	0.48
1:D:673:PHE:CE2	1:D:698:ILE:HD11	2.48	0.48
1:B:653:ARG:HD3	1:B:660:PHE:HB2	1.95	0.48
1:D:606:LEU:O	1:D:653:ARG:HD2	2.14	0.48
1:C:724:TYR:HB3	1:C:726:TRP:CH2	2.49	0.48
1:C:255:PRO:HB2	1:C:327:LYS:HD3	1.94	0.48
1:B:612:LYS:NZ	1:B:736:LEU:HD22	2.27	0.48
1:A:503:TRP:H	1:A:516:HIS:HD2	1.61	0.48
1:C:387:ASP:N	1:C:387:ASP:OD1	2.45	0.48
1:A:456:PHE:CE1	1:A:752:HIS:HE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:HIS:NE2	1:A:732:LYS:HE2	2.30	0.47
1:B:11:TRP:CE2	1:B:58:PRO:HG3	2.49	0.47
1:A:753:HIS:HB3	1:B:220:HIS:CD2	2.50	0.47
1:A:736:LEU:N	1:A:737:PRO:HD3	2.29	0.47
1:B:606:LEU:HD21	1:B:609:VAL:HG22	1.95	0.47
1:C:72:ALA:HB1	1:C:105:ILE:HD11	1.87	0.47
1:B:29:GLU:O	1:B:33:GLY:N	2.41	0.47
1:B:11:TRP:CD2	1:B:58:PRO:HG3	2.49	0.47
1:C:66:ASP:HB3	1:C:331:MET:HE2	1.97	0.47
1:A:65:HIS:HA	1:A:68:PHE:HD2	1.80	0.47
1:B:724:TYR:CB	1:B:726:TRP:CH2	2.98	0.47
1:A:387:ASP:N	1:A:387:ASP:OD1	2.48	0.47
1:C:593:GLU:O	1:C:597:LYS:HG3	2.15	0.47
1:D:66:ASP:CB	1:D:331:MET:HE2	2.45	0.47
1:D:726:TRP:HB3	1:D:727:PRO:HD2	1.97	0.47
1:B:735:ILE:HG23	1:B:735:ILE:O	2.16	0.46
1:C:77:LEU:HB2	1:C:105:ILE:HG23	1.97	0.46
1:A:591:LEU:HD12	1:A:592:GLN:N	2.30	0.46
1:C:520:THR:HG21	1:C:574:LEU:HD13	1.97	0.46
1:C:604:SER:O	1:C:658:ARG:NH1	2.48	0.46
1:B:7:LYS:HD3	1:B:35:LYS:HD3	1.98	0.46
1:C:171:LYS:HG2	1:C:173:GLU:HG2	1.97	0.46
1:A:166:GLY:O	1:A:186:ASN:ND2	2.47	0.46
1:D:387:ASP:N	1:D:387:ASP:OD1	2.45	0.46
1:B:400:TYR:HB2	1:B:407:PRO:HA	1.98	0.46
1:A:257:LYS:CE	1:A:329:GLU:OE1	2.63	0.46
1:D:26:LYS:HA	1:D:26:LYS:HD3	1.73	0.46
1:C:96:ASP:OD1	1:C:99:ARG:NH2	2.48	0.46
1:A:646:ILE:HB	1:A:647:PRO:HD3	1.97	0.46
1:A:722:LYS:HG2	1:A:723:GLU:N	2.31	0.46
1:A:635:HIS:NE2	1:A:732:LYS:HG3	2.31	0.46
1:C:708:MET:HG2	1:C:726:TRP:CZ2	2.50	0.46
1:A:735:ILE:HG22	1:A:735:ILE:O	2.15	0.46
1:B:315:ASP:HB3	1:B:318:ILE:HG12	1.98	0.46
1:B:133:ILE:N	1:B:134:PRO:CD	2.79	0.46
1:B:606:LEU:HD21	1:B:609:VAL:CG2	2.46	0.46
1:D:171:LYS:HE2	1:D:173:GLU:CD	2.36	0.46
1:A:450:THR:HG22	1:A:531:PRO:HA	1.97	0.46
1:C:450:THR:HG22	1:C:531:PRO:HA	1.97	0.45
1:C:184:VAL:HG23	1:C:366:GLN:HB2	1.98	0.45
1:A:442:ASN:OD1	1:A:447:PHE:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:HIS:HE1	1:D:606:LEU:HD21	1.79	0.45
1:A:32:THR:HG22	1:A:34:ILE:HD13	1.98	0.45
1:A:11:TRP:CE2	1:A:58:PRO:HG3	2.51	0.45
1:C:159:TRP:N	1:C:160:PRO:CD	2.80	0.45
1:C:21:LEU:CD1	1:C:285:LEU:HD13	2.46	0.45
1:C:618:LEU:HD12	1:C:633:SER:HB2	1.98	0.45
1:D:736:LEU:HB2	1:D:737:PRO:HD3	1.97	0.45
1:C:653:ARG:HG2	1:C:658:ARG:HB2	1.98	0.45
1:B:584:ILE:O	1:B:591:LEU:CD1	2.65	0.45
1:C:86:PHE:HZ	1:C:286:LEU:HD13	1.81	0.45
1:A:612:LYS:HD2	1:A:736:LEU:HD22	1.98	0.45
1:C:22:ALA:O	1:C:26:LYS:HG3	2.17	0.45
1:C:69:GLY:HA3	1:C:333:ASN:O	2.17	0.45
1:B:692:HIS:CG	1:B:692:HIS:O	2.68	0.45
1:D:661:THR:O	1:D:661:THR:HG23	2.16	0.44
1:D:555:ASN:CB	1:D:605:ASN:HB2	2.45	0.44
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.52	0.44
1:D:650:LEU:HD23	1:D:654:LEU:HD12	2.00	0.44
1:B:442:ASN:HA	1:B:445:HIS:O	2.18	0.44
1:D:502:SER:HA	1:D:516:HIS:HD2	1.83	0.44
1:B:152:LEU:HD11	1:B:205:MET:HE3	2.00	0.44
1:D:579:ARG:NE	1:D:579:ARG:HA	2.32	0.44
1:B:387:ASP:OD1	1:B:387:ASP:N	2.50	0.44
1:A:585:PHE:HA	1:A:591:LEU:HD21	2.00	0.44
1:C:626:ILE:HG22	1:C:627:ARG:N	2.33	0.44
1:D:177:TYR:CZ	1:D:332:PRO:HG3	2.53	0.44
1:B:413:MET:HE1	1:B:473:PRO:C	2.39	0.43
1:C:259:PHE:HB3	1:C:331:MET:CG	2.47	0.43
1:C:700:LEU:HD22	1:C:704:PHE:CE2	2.53	0.43
1:C:616:ASP:OD1	1:C:617:ASP:N	2.45	0.43
1:C:179:ILE:HG13	1:C:180:LYS:N	2.33	0.43
1:C:445:HIS:HA	1:C:752:HIS:HB3	2.00	0.43
1:A:635:HIS:CE1	1:A:732:LYS:HE2	2.53	0.43
1:D:516:HIS:CE1	1:D:545:THR:HG22	2.53	0.43
1:B:184:VAL:CG2	1:B:366:GLN:HB2	2.48	0.43
1:D:32:THR:HG22	1:D:34:ILE:HD13	2.00	0.43
1:C:77:LEU:HB2	1:C:105:ILE:CG2	2.48	0.43
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.54	0.43
1:B:712:LEU:CD1	1:B:714:ASP:H	2.31	0.43
1:C:682:PHE:CE1	1:C:697:GLN:HB2	2.54	0.43
1:B:722:LYS:HD3	1:B:724:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLY:HA3	1:B:333:ASN:O	2.19	0.43
1:A:516:HIS:CE1	1:A:545:THR:HG22	2.53	0.43
1:B:712:LEU:HD12	1:B:713:GLU:CA	2.45	0.43
1:C:723:GLU:OE1	1:C:732:LYS:HG2	2.18	0.43
1:C:376:ALA:CB	1:C:530:THR:HG22	2.48	0.43
1:A:462:PHE:HB2	1:A:481:MET:HE3	2.01	0.43
1:A:675:SER:OG	1:A:676:THR:N	2.51	0.43
1:D:554:TRP:HB2	1:D:599:ILE:HG22	2.01	0.42
1:D:476:TRP:N	1:D:477:PRO:CD	2.82	0.42
1:A:413:MET:HG2	1:A:430:TYR:CD2	2.53	0.42
1:A:736:LEU:N	1:A:737:PRO:CD	2.82	0.42
1:D:476:TRP:CG	1:D:477:PRO:HD3	2.54	0.42
1:D:635:HIS:CE1	1:D:732:LYS:HG3	2.54	0.42
1:A:177:TYR:CZ	1:A:332:PRO:HG3	2.54	0.42
1:A:718:ALA:HB1	1:A:722:LYS:HE2	2.01	0.42
1:B:726:TRP:HB3	1:B:727:PRO:HD2	1.99	0.42
1:B:177:TYR:CZ	1:B:332:PRO:HG3	2.55	0.42
1:B:597:LYS:HA	1:B:600:GLU:HG2	2.01	0.42
1:D:682:PHE:CE2	1:D:697:GLN:NE2	2.87	0.42
1:C:237:ASP:O	1:C:240:LYS:HD3	2.20	0.42
1:B:712:LEU:HD12	1:B:714:ASP:H	1.85	0.42
1:D:184:VAL:HG23	1:D:366:GLN:HB2	2.01	0.42
1:C:653:ARG:HG2	1:C:658:ARG:CB	2.50	0.42
1:B:384:LEU:HD12	1:B:525:MET:SD	2.60	0.42
1:A:635:HIS:CE1	1:A:732:LYS:CE	3.03	0.42
1:B:415:ARG:NH1	1:B:426:GLU:OE2	2.51	0.42
1:C:476:TRP:N	1:C:477:PRO:CD	2.83	0.42
1:B:500:HIS:HD2	1:B:548:LEU:HD11	1.85	0.42
1:C:32:THR:HG22	1:C:34:ILE:HD13	2.02	0.41
1:A:159:TRP:N	1:A:160:PRO:CD	2.82	0.41
1:A:476:TRP:N	1:A:477:PRO:CD	2.83	0.41
1:A:491:SER:O	1:A:492:GLU:HB2	2.20	0.41
1:D:696:LEU:HD21	1:D:698:ILE:CG2	2.50	0.41
1:C:594:ARG:HA	1:C:597:LYS:HD2	2.02	0.41
1:C:606:LEU:O	1:C:653:ARG:HD2	2.21	0.41
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.55	0.41
1:C:177:TYR:CE1	1:C:332:PRO:HG3	2.55	0.41
1:C:202:ASN:HB2	1:C:204:HIS:CD2	2.55	0.41
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.56	0.41
1:C:424:ILE:HD11	1:C:572:PRO:HB2	2.03	0.41
1:D:400:TYR:HB2	1:D:407:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:OD1	1:A:374:LEU:CD2	2.69	0.41
1:C:611:ALA:HB2	2:G:337:LEU:HD12	2.02	0.41
1:C:99:ARG:HG3	1:C:104:LEU:CD2	2.50	0.41
1:B:516:HIS:HE1	1:B:545:THR:HG22	1.85	0.41
1:B:123:LEU:HD13	1:B:136:LEU:HD11	2.02	0.41
1:B:646:ILE:HB	1:B:647:PRO:HD3	2.03	0.41
1:D:626:ILE:HG22	1:D:627:ARG:N	2.36	0.41
1:C:400:TYR:CE2	1:C:751:HIS:HD2	2.39	0.41
1:B:159:TRP:N	1:B:160:PRO:CD	2.84	0.41
1:A:397:ILE:H	1:A:397:ILE:HD12	1.86	0.41
1:A:315:ASP:HB3	1:A:318:ILE:HG12	2.03	0.41
1:D:376:ALA:CB	1:D:530:THR:HG22	2.51	0.41
1:A:500:HIS:HE1	1:A:606:LEU:HD21	1.86	0.41
1:B:171:LYS:HE2	1:B:173:GLU:HG3	2.03	0.41
1:D:615:TRP:HZ2	1:D:694:PRO:HA	1.86	0.41
1:B:40:HIS:CG	1:B:40:HIS:O	2.74	0.41
1:D:648:LEU:O	1:D:652:GLY:CA	2.68	0.41
1:A:442:ASN:HA	1:A:445:HIS:O	2.21	0.41
1:C:400:TYR:HB2	1:C:407:PRO:HA	2.04	0.41
1:B:723:GLU:OE1	1:B:732:LYS:CG	2.69	0.41
1:B:476:TRP:N	1:B:477:PRO:CD	2.84	0.41
1:C:588:ASP:HB3	1:C:591:LEU:HD12	2.02	0.41
1:A:612:LYS:HD2	1:A:736:LEU:CD2	2.51	0.40
1:A:476:TRP:CG	1:A:477:PRO:HD3	2.56	0.40
1:B:197:VAL:HG12	1:B:201:LYS:NZ	2.37	0.40
1:B:82:PRO:HG2	1:B:95:TRP:CH2	2.57	0.40
1:B:220:HIS:HB2	1:B:222:GLU:OE2	2.21	0.40
1:B:638:PHE:CD2	1:B:731:LEU:HD11	2.56	0.40
1:A:98:VAL:HG21	1:A:108:PRO:HD3	2.04	0.40
1:A:593:GLU:HG2	1:A:597:LYS:HE3	2.03	0.40
1:B:391:PRO:HG3	1:B:414:TYR:CE2	2.55	0.40
1:A:260:VAL:HB	1:A:330:ILE:HA	2.02	0.40
1:B:93:PHE:O	1:B:96:ASP:HB2	2.21	0.40
1:C:56:ASP:OD1	1:C:56:ASP:N	2.54	0.40
1:A:612:LYS:CD	1:A:736:LEU:HD22	2.51	0.40
1:A:140:LEU:HD23	1:A:143:LYS:HE3	2.04	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	726/753 (96%)	702 (97%)	22 (3%)	2 (0%)	46 79
1	B	705/753 (94%)	691 (98%)	14 (2%)	0	100 100
1	C	717/753 (95%)	703 (98%)	14 (2%)	0	100 100
1	D	722/753 (96%)	707 (98%)	15 (2%)	0	100 100
2	E	6/17 (35%)	6 (100%)	0	0	100 100
2	F	6/17 (35%)	6 (100%)	0	0	100 100
2	G	6/17 (35%)	6 (100%)	0	0	100 100
2	H	6/17 (35%)	6 (100%)	0	0	100 100
All	All	2894/3080 (94%)	2827 (98%)	65 (2%)	2 (0%)	56 87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	679	GLU
1	A	678	VAL

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	608/626 (97%)	603 (99%)	5 (1%)	86 97
1	B	593/626 (95%)	591 (100%)	2 (0%)	94 99
1	C	600/626 (96%)	598 (100%)	2 (0%)	94 99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	605/626 (97%)	601 (99%)	4 (1%)	88 97
2	E	6/12 (50%)	6 (100%)	0	100 100
2	F	6/12 (50%)	6 (100%)	0	100 100
2	G	6/12 (50%)	5 (83%)	1 (17%)	3 8
2	H	6/12 (50%)	6 (100%)	0	100 100
All	All	2430/2552 (95%)	2416 (99%)	14 (1%)	90 98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	THR
1	A	384	LEU
1	A	579	ARG
1	A	752	HIS
1	B	327	LYS
1	B	747	GLU
1	C	653	ARG
1	C	695	TRP
1	D	355	ARG
1	D	665	ILE
1	D	715	LEU
1	D	734	SER
2	G	333	SER

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

Mol	Chain	Res	Type
1	A	500	HIS
1	A	516	HIS
1	A	748	HIS
1	A	749	HIS
1	A	752	HIS
1	B	273	ASN
1	B	423	ASN
1	B	516	HIS
1	C	204	HIS
1	C	350	ASN
1	C	516	HIS

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Mol	Chain	Res	Type
1	D	220	HIS
1	D	500	HIS
1	D	516	HIS
1	D	656	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	MAL	A	900	-	24,24,24	0.53	0	35,35,35	0.58	0
3	MAL	B	900	-	24,24,24	0.53	0	35,35,35	0.62	0
3	MAL	C	900	-	24,24,24	0.53	0	35,35,35	0.68	0
3	MAL	D	900	-	24,24,24	0.55	0	35,35,35	0.90	1 (2%)

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
3	MAL	A	900	-	-	0/8/48/48	0/2/2/2
3	MAL	B	900	-	-	0/8/48/48	0/2/2/2
3	MAL	C	900	-	-	0/8/48/48	0/2/2/2
3	MAL	D	900	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	900	MAL	C1'-C2'-C3'	2.97	114.84	110.43

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 (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	734/753 (97%)	-0.25	9 (1%) 81 73	49, 79, 122, 165	0
1	B	717/753 (95%)	-0.08	29 (4%) 42 30	51, 92, 163, 199	0
1	C	725/753 (96%)	0.08	43 (5%) 26 16	54, 109, 174, 214	0
1	D	730/753 (96%)	-0.18	18 (2%) 61 48	46, 83, 142, 217	0
2	E	8/17 (47%)	-0.10	0 100 100	63, 73, 93, 94	0
2	F	8/17 (47%)	0.25	1 (12%) 5 2	89, 96, 118, 120	0
2	G	8/17 (47%)	-0.07	0 100 100	76, 88, 99, 108	0
2	H	8/17 (47%)	-0.30	0 100 100	77, 82, 96, 101	0
All	All	2938/3080 (95%)	-0.11	100 (3%) 49 36	46, 88, 158, 217	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	703	GLU	10.7
1	A	1	MET	7.1
1	C	710	GLU	6.0
1	B	614	ALA	5.9
1	C	709	LEU	5.8
1	B	712	LEU	5.2
1	C	711	ASP	5.1
1	B	615	TRP	5.0
1	C	300	LEU	4.9
1	C	594	ARG	4.8
1	C	704	PHE	4.8
1	B	734	SER	4.7
1	B	638	PHE	4.7
1	C	650	LEU	4.6
1	B	738	ASP	4.3
1	B	636	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	713	GLU	4.2
1	D	630	GLN	4.0
1	B	37	THR	3.9
1	C	632	GLU	3.9
1	C	646	ILE	3.8
1	B	670	ALA	3.7
1	C	708	MET	3.7
1	B	613	CYS	3.7
1	C	595	VAL	3.7
1	D	682	PHE	3.7
1	C	569	ALA	3.7
1	C	446	GLU	3.6
1	B	708	MET	3.6
1	C	105	ILE	3.6
1	C	701	THR	3.6
1	C	591	LEU	3.5
1	C	734	SER	3.5
1	D	627	ARG	3.4
1	C	634	VAL	3.4
1	A	3	THR	3.4
1	B	679	GLU	3.3
1	B	682	PHE	3.3
1	D	597	LYS	3.3
1	D	748	HIS	3.2
1	C	584	ILE	3.2
1	C	702	GLU	3.2
1	D	629	ARG	3.2
1	C	599	ILE	3.1
1	C	548	LEU	3.1
1	B	668	ASP	3.0
1	C	549	HIS	3.0
1	D	631	LEU	3.0
1	D	519	LEU	2.9
1	B	568	ILE	2.9
1	C	174	ASN	2.8
1	B	709	LEU	2.8
1	D	569	ALA	2.8
1	B	612	LYS	2.8
1	D	611	ALA	2.8
1	C	552	GLN	2.7
1	C	732	LYS	2.7
1	B	663	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	705	VAL	2.7
1	C	659	HIS	2.7
1	C	79	GLU	2.6
1	B	698	ILE	2.6
1	D	643	GLY	2.6
1	C	8	LEU	2.5
1	C	7	LYS	2.5
1	C	565	THR	2.5
1	A	627	ARG	2.5
1	B	683	ALA	2.5
1	D	568	ILE	2.5
2	F	334	TYR	2.4
1	D	747	GLU	2.4
1	C	111	VAL	2.4
1	D	734	SER	2.4
1	A	285	LEU	2.4
1	C	563	LEU	2.4
1	C	654	LEU	2.4
1	A	721	PRO	2.3
1	C	501	VAL	2.3
1	D	626	ILE	2.3
1	D	666	THR	2.3
1	B	637	LYS	2.3
1	C	707	LYS	2.3
1	C	518	LEU	2.2
1	C	722	LYS	2.2
1	B	673	PHE	2.2
1	D	673	PHE	2.2
1	A	4	GLU	2.2
1	A	495	PHE	2.1
1	A	300	LEU	2.1
1	C	245	VAL	2.1
1	B	669	MET	2.1
1	B	646	ILE	2.1
1	B	511	GLU	2.1
1	B	555	ASN	2.1
1	C	140	LEU	2.1
1	D	614	ALA	2.1
1	C	312	LEU	2.1
1	B	648	LEU	2.1
1	B	551	ALA	2.0
1	A	704	PHE	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
3	MAL	C	900	23/23	0.94	0.17	0.03	61,77,85,94	0
3	MAL	D	900	23/23	0.96	0.16	-0.02	47,59,69,73	0
4	ZN	C	910	1/1	0.99	0.17	-0.07	57,57,57,57	0
4	ZN	B	910	1/1	0.99	0.17	-0.18	75,75,75,75	0
3	MAL	B	900	23/23	0.96	0.18	-0.21	50,59,76,93	0
4	ZN	D	910	1/1	1.00	0.14	-0.66	74,74,74,74	0
3	MAL	A	900	23/23	0.97	0.14	-1.04	48,58,73,84	0
4	ZN	A	910	1/1	0.79	0.13	-1.32	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.