



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2023 – 05:51 PM EST

PDB ID : 3EUA
Title : CRYSTAL STRUCTURE OF A PUTATIVE PHOSPHOSUGAR ISOMERASE (BSU32610) FROM BACILLUS SUBTILIS AT 1.90 Å RESOLUTION
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-10-09
Resolution : 1.90 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

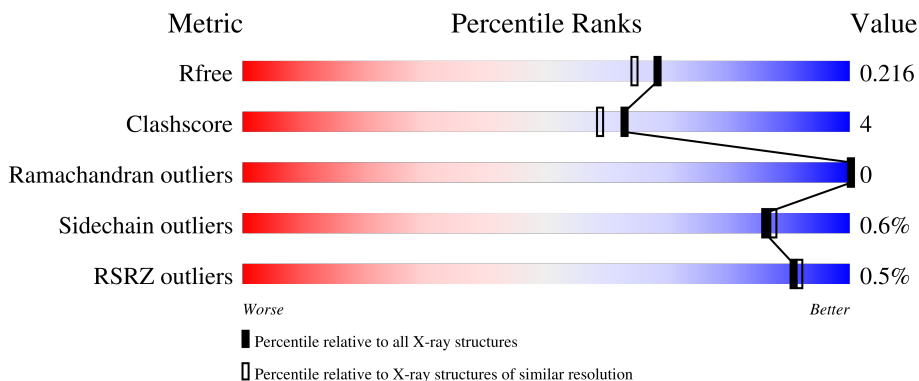
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




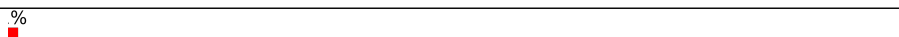
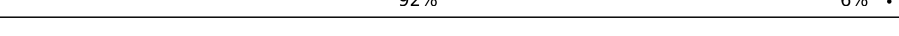
The reported resolution of this entry is 1.90 Å.

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.



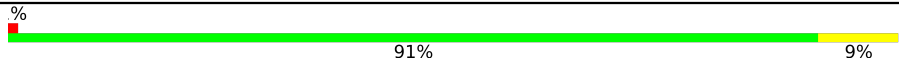
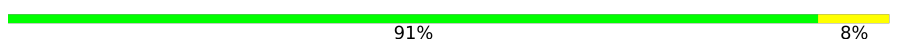

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	329	 91% 8% .
1	B	329	 91% 7% .
1	C	329	 90% 8% ..
1	D	329	 92% 6% .
1	E	329	 92% 6% .

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Mol	Chain	Length	Quality of chain
1	F	329	 % 91% 9%
1	G	329	 91% 8%
1	H	329	 % 92% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22425 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 PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	325	Total 2574	C 1648	N 425	O 491	S 3	Se 7	0	2	0
1	B	324	Total 2560	C 1642	N 421	O 486	S 3	Se 8	0	3	0
1	C	324	Total 2578	C 1652	N 425	O 490	S 3	Se 8	0	3	0
1	D	324	Total 2579	C 1656	N 427	O 485	S 3	Se 8	0	4	0
1	E	324	Total 2567	C 1648	N 424	O 485	S 3	Se 7	0	3	0
1	F	329	Total 2619	C 1677	N 431	O 499	S 3	Se 9	0	4	0
1	G	328	Total 2608	C 1670	N 432	O 495	S 3	Se 8	0	3	0
1	H	327	Total 2594	C 1663	N 428	O 493	S 3	Se 7	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

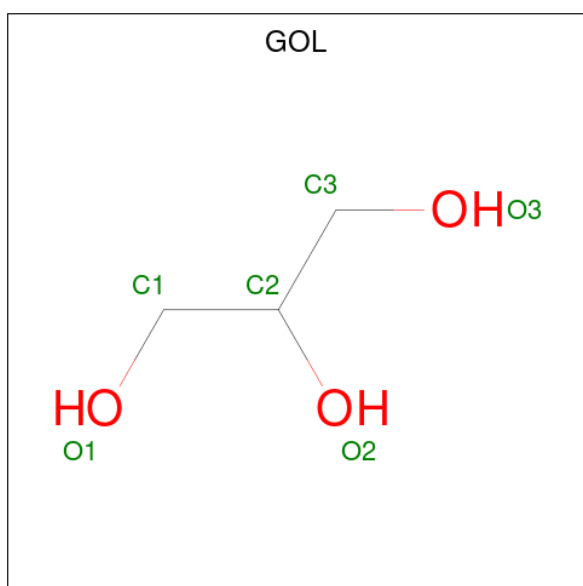
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O32157
B	0	GLY	-	expression tag	UNP O32157
C	0	GLY	-	expression tag	UNP O32157
D	0	GLY	-	expression tag	UNP O32157
E	0	GLY	-	expression tag	UNP O32157
F	0	GLY	-	expression tag	UNP O32157
G	0	GLY	-	expression tag	UNP O32157
H	0	GLY	-	expression tag	UNP O32157

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		


- Molecule 4 is water.

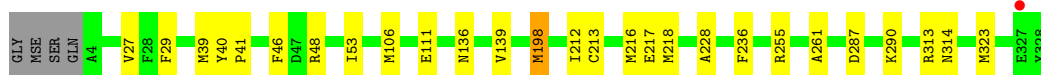
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	165	Total O 167 167	0	2
4	B	176	Total O 177 177	0	1
4	C	175	Total O 175 175	0	0
4	D	157	Total O 158 158	0	1
4	E	179	Total O 180 180	0	1
4	F	193	Total O 194 194	0	1
4	G	180	Total O 180 180	0	0
4	H	477	Total O 477 477	0	0

3 Residue-property plots [i](#)

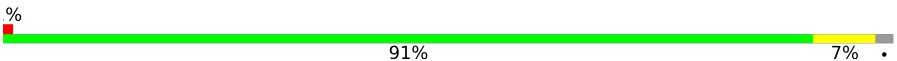
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE

Chain A: 




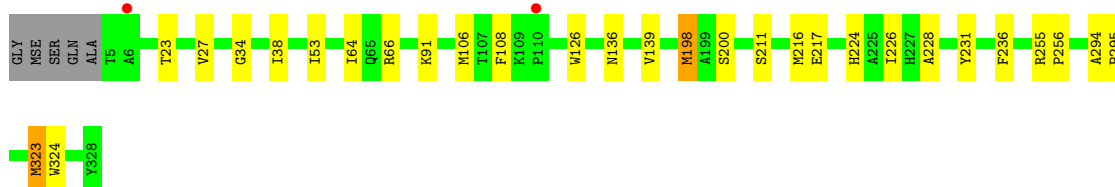
- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE

Chain B: 

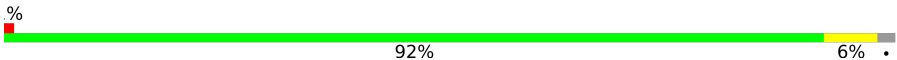


- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE

Chain C: 



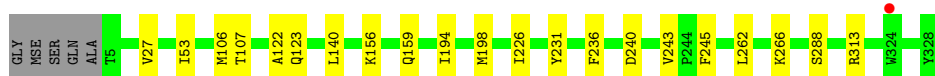
- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE

Chain D: 

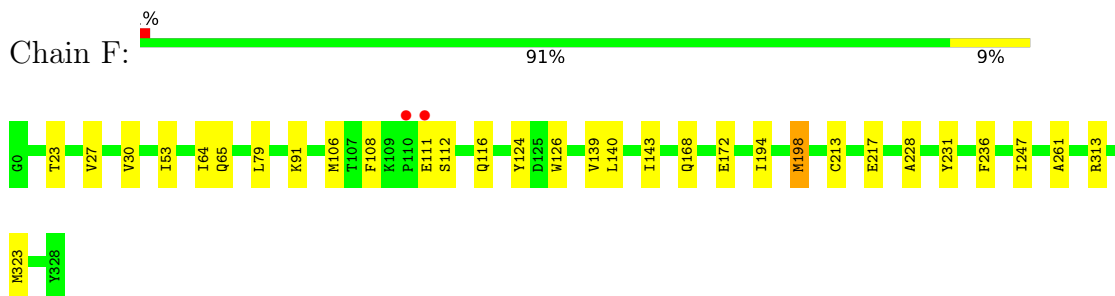


- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE

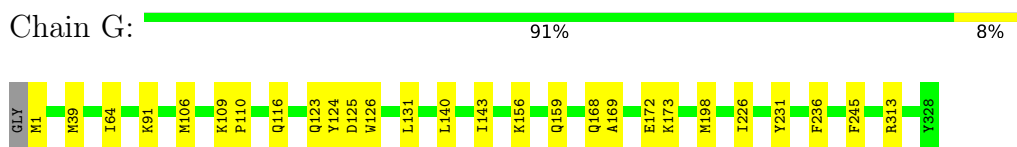
Chain E: 



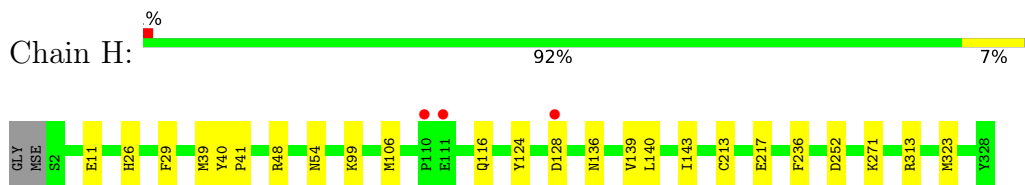
- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE



- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE



- Molecule 1: PUTATIVE FRUCTOSE-AMINOACID-6-PHOSPHATE DEGLYCASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.86Å 91.82Å 119.04Å 109.30° 100.45° 96.55°	Depositor
Resolution (Å)	29.98 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.98-1.90) 97.1 (29.97-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.168 , 0.212 0.175 , 0.216	Depositor DCC
R_{free} test set	8990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,h+k+l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22425	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9555e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FLC

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	0.71	1/2626 (0.0%)	0.81	4/3549 (0.1%)
1	B	0.70	0/2612	0.80	2/3531 (0.1%)
1	C	0.74	1/2630 (0.0%)	0.81	2/3552 (0.1%)
1	D	0.75	1/2631 (0.0%)	0.80	0/3553
1	E	0.77	0/2619	0.83	2/3539 (0.1%)
1	F	0.83	3/2670 (0.1%)	0.83	1/3602 (0.0%)
1	G	0.79	1/2660 (0.0%)	0.85	2/3591 (0.1%)
1	H	0.77	1/2646 (0.0%)	0.85	3/3575 (0.1%)
All	All	0.76	8/21094 (0.0%)	0.82	16/28492 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	GLU	CG-CD	6.79	1.62	1.51
1	H	11	GLU	CD-OE1	6.62	1.32	1.25
1	C	198	MSE	SE-CE	-6.08	1.59	1.95
1	A	111	GLU	CG-CD	5.84	1.60	1.51
1	F	198[A]	MSE	SE-CE	-5.78	1.61	1.95
1	F	198[B]	MSE	SE-CE	-5.78	1.61	1.95
1	D	126	TRP	CB-CG	-5.55	1.40	1.50
1	G	126	TRP	CB-CG	-5.50	1.40	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	252	ASP	CB-CG-OD1	7.71	125.24	118.30
1	E	313	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	F	313	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	G	1	MSE	N-CA-C	6.19	127.72	111.00
1	E	313	ARG	NE-CZ-NH2	-6.15	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	48	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	198	MSE	CG-SE-CE	-5.69	86.39	98.90
1	B	313	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	G	313	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	48	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	313	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	313	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	313	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	66	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	198	MSE	CG-SE-CE	-5.26	87.33	98.90
1	A	255	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2490	26	0
1	B	2560	0	2470	24	0
1	C	2578	0	2500	29	0
1	D	2579	0	2505	18	0
1	E	2567	0	2494	19	0
1	F	2619	0	2544	31	0
1	G	2608	0	2538	22	0
1	H	2594	0	2513	17	0
2	C	13	0	5	0	0
2	H	13	0	5	0	0
3	C	6	0	8	0	0
3	H	6	0	8	0	0
4	A	167	0	0	0	0
4	B	177	0	0	1	0
4	C	175	0	0	0	0
4	D	158	0	0	0	0
4	E	180	0	0	0	0
4	F	194	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	180	0	0	4	0
4	H	477	0	0	2	0
All	All	22425	0	20080	174	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 4.

All (174) 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:E:106[B]:MSE:SE	1:E:106[B]:MSE:CE	2.20	1.40
1:F:198[A]:MSE:HE3	1:F:228:ALA:HA	1.30	1.13
1:B:198:MSE:HE3	1:B:226:ILE:HB	1.32	1.09
1:A:198:MSE:HE3	1:A:228:ALA:HA	1.36	1.06
1:G:198:MSE:HE2	1:G:226:ILE:HB	1.47	0.94
1:A:198:MSE:CE	1:A:261:ALA:HB1	1.99	0.91
1:B:198:MSE:CE	1:B:226:ILE:CG2	2.49	0.91
1:B:271:LYS:NZ	1:C:23:THR:HG21	1.85	0.91
1:A:212:ILE:HA	1:A:216[B]:MSE:HE3	1.55	0.89
1:A:198:MSE:HE1	1:A:261:ALA:HB1	1.54	0.89
1:B:198:MSE:HE3	1:B:226:ILE:CB	2.02	0.88
1:D:106:MSE:HE2	1:D:124:TYR:HD2	1.38	0.86
1:F:198[A]:MSE:HE2	1:F:261:ALA:CB	2.05	0.86
1:A:198:MSE:CE	1:A:261:ALA:CB	2.54	0.86
1:E:198:MSE:HE2	1:E:226:ILE:HB	1.58	0.86
1:F:198[A]:MSE:HE2	1:F:261:ALA:HB1	1.56	0.85
1:E:198:MSE:HE1	1:E:231:TYR:CD1	2.12	0.85
1:A:198:MSE:HE1	1:A:261:ALA:CB	2.05	0.84
1:H:106[B]:MSE:HE1	1:H:140:LEU:HA	1.59	0.84
1:F:106[B]:MSE:HE1	1:F:140:LEU:HA	1.60	0.83
1:C:198:MSE:HE1	1:C:226:ILE:HG22	1.58	0.83
1:B:198:MSE:HE1	1:B:226:ILE:CG2	2.11	0.81
1:B:198:MSE:CE	1:B:226:ILE:HG22	2.11	0.80
1:F:198[A]:MSE:CE	1:F:261:ALA:HB1	2.13	0.79
1:C:198:MSE:HE1	1:C:226:ILE:CG2	2.13	0.78
1:D:106:MSE:HE2	1:D:124:TYR:CD2	2.19	0.78
1:C:198:MSE:HE3	1:C:226:ILE:HB	1.67	0.76
1:C:198:MSE:CE	1:C:226:ILE:HG22	2.15	0.76
1:A:198:MSE:HE3	1:A:228:ALA:CA	2.14	0.76
1:F:106[B]:MSE:HE2	1:F:139:VAL:HG12	1.68	0.74
1:A:217:GLU:OE2	1:A:323:MSE:HE1	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG23	1:A:53:ILE:HG21	1.71	0.71
1:B:198:MSE:HE1	1:B:226:ILE:HG21	1.72	0.71
1:G:64:ILE:HD13	1:G:91:LYS:HE3	1.74	0.70
1:E:198:MSE:HE2	1:E:226:ILE:CB	2.21	0.69
1:E:106[B]:MSE:HE1	1:E:140:LEU:HD13	1.75	0.68
1:C:198:MSE:CE	1:C:226:ILE:CG2	2.71	0.67
1:A:198:MSE:HE2	1:A:261:ALA:HB1	1.76	0.67
1:A:198:MSE:HE2	1:A:261:ALA:CB	2.22	0.67
1:H:106[B]:MSE:HE1	1:H:140:LEU:CA	2.25	0.67
1:F:198[A]:MSE:CE	1:F:261:ALA:CB	2.72	0.67
1:D:27[A]:VAL:HG23	1:D:53:ILE:HG21	1.77	0.67
1:G:198:MSE:HE1	1:G:231:TYR:CD1	2.29	0.66
1:C:198:MSE:HE1	1:C:231:TYR:HB2	1.77	0.66
1:D:212:ILE:HA	1:D:216[B]:MSE:HE3	1.77	0.65
1:F:198[B]:MSE:HE2	1:F:247:ILE:HG12	1.78	0.65
1:A:216[B]:MSE:HE1	1:B:224:HIS:HE1	1.62	0.64
1:C:217:GLU:OE2	1:C:323[B]:MSE:HE1	1.96	0.64
1:F:168:GLN:O	1:F:172:GLU:HG2	1.97	0.64
1:A:314[B]:ASN:ND2	1:D:153:ASN:OD1	2.30	0.63
1:G:110:PRO:HB3	1:G:123[A]:GLN:NE2	2.14	0.63
1:H:106[B]:MSE:CE	1:H:143:ILE:HD12	2.29	0.63
1:F:198[A]:MSE:HE1	1:F:231:TYR:CD2	2.34	0.62
1:D:106:MSE:HE1	1:D:136:ASN:HA	1.81	0.62
1:F:106[B]:MSE:HE1	1:F:140:LEU:CA	2.28	0.62
1:H:116:GLN:NE2	4:H:803:HOH:O	2.32	0.62
1:C:198:MSE:HE2	1:C:228:ALA:HA	1.82	0.62
1:F:198[B]:MSE:HE2	1:F:247:ILE:CG1	2.30	0.62
1:E:198:MSE:HE1	1:E:231:TYR:CE1	2.36	0.61
1:G:106[B]:MSE:HE1	1:G:140:LEU:HA	1.82	0.61
1:A:216[B]:MSE:HE1	1:B:224:HIS:CE1	2.36	0.60
1:E:198:MSE:HE3	1:E:245:PHE:HE2	1.66	0.60
1:G:106[B]:MSE:HE2	1:G:143:ILE:HD12	1.82	0.60
1:G:198:MSE:HE2	1:G:226:ILE:CB	2.26	0.60
1:F:64:ILE:HD13	1:F:91:LYS:HE3	1.84	0.59
1:F:106[B]:MSE:CE	1:F:143:ILE:HD12	2.32	0.59
1:E:198:MSE:HE3	1:E:245:PHE:CE2	2.38	0.59
1:B:271:LYS:HZ1	1:C:23:THR:HG21	1.66	0.58
1:G:131:LEU:HD22	1:G:168:GLN:HG2	1.85	0.58
1:H:217:GLU:OE2	1:H:323:MSE:HE1	2.03	0.58
1:F:198[B]:MSE:HE2	1:F:247:ILE:CG2	2.34	0.57
1:C:106:MSE:HE3	1:C:139:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD1	1:A:290:LYS:HE2	2.06	0.56
1:H:106[B]:MSE:HE2	1:H:143:ILE:HD12	1.86	0.56
1:G:198:MSE:HE1	1:G:231:TYR:CE1	2.41	0.55
1:H:106[B]:MSE:HE2	1:H:139:VAL:HG12	1.86	0.55
1:C:224:HIS:HE1	1:D:216[B]:MSE:HE1	1.71	0.55
1:C:27:VAL:HG23	1:C:53:ILE:HG21	1.88	0.55
1:F:65:GLN:NE2	4:F:1054:HOH:O	2.36	0.54
1:A:198:MSE:HE1	1:A:261:ALA:HB2	1.86	0.54
1:C:198:MSE:HE3	1:C:226:ILE:CB	2.36	0.54
1:G:169:ALA:O	1:G:173:LYS:HG3	2.08	0.54
1:H:106[B]:MSE:HG2	1:H:124:TYR:HD2	1.73	0.54
1:C:106:MSE:HE3	1:C:139:VAL:HG12	1.88	0.54
1:F:198[B]:MSE:HE2	1:F:247:ILE:HG23	1.90	0.54
1:D:106:MSE:CE	1:D:139:VAL:HB	2.38	0.53
1:A:27:VAL:HG23	1:A:53:ILE:CG2	2.39	0.52
1:H:213:CYS:O	1:H:217:GLU:HB3	2.10	0.52
1:C:224:HIS:CE1	1:D:216[B]:MSE:HE1	2.46	0.51
1:F:106[B]:MSE:HG2	1:F:124:TYR:HD2	1.77	0.50
1:C:200:SER:HB3	1:C:228:ALA:HB3	1.93	0.50
1:F:198[B]:MSE:CE	1:F:247:ILE:HG23	2.42	0.49
1:G:106[B]:MSE:HE1	1:G:140:LEU:CA	2.43	0.49
1:H:106[A]:MSE:HE1	1:H:136:ASN:O	2.12	0.49
1:B:198:MSE:HE1	1:B:231:TYR:CD1	2.48	0.48
1:B:303:ARG:HA	1:B:303:ARG:HD3	1.70	0.48
1:D:106:MSE:CE	1:D:124:TYR:CD2	2.95	0.48
1:F:106[B]:MSE:CE	1:F:139:VAL:HG12	2.42	0.48
1:F:27:VAL:HG23	1:F:53:ILE:HG21	1.96	0.47
1:B:108:PHE:CE1	1:B:126:TRP:HB3	2.49	0.47
1:B:45:VAL:HG22	1:B:292:TYR:CD1	2.50	0.47
1:E:198:MSE:CE	1:E:245:PHE:HE2	2.27	0.47
1:G:116:GLN:NE2	4:G:1580:HOH:O	2.44	0.47
1:A:106:MSE:HE3	1:A:139:VAL:HG12	1.96	0.46
1:H:26:HIS:CE1	1:H:54:ASN:ND2	2.84	0.46
1:F:198[A]:MSE:HE1	1:F:231:TYR:CG	2.49	0.46
1:A:106:MSE:HE3	1:A:139:VAL:CG1	2.46	0.46
1:G:39:MSE:HG2	1:G:140:LEU:HD21	1.96	0.46
1:B:244:PRO:HG3	1:B:271:LYS:HD3	1.98	0.46
1:B:323[B]:MSE:HG3	1:B:324:TRP:CD2	2.50	0.46
1:D:169:ALA:O	1:D:173:LYS:HG3	2.14	0.46
1:D:106:MSE:HE3	1:D:139:VAL:CG1	2.46	0.46
1:H:29:PHE:HB3	1:H:39:MSE:SE	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:CYS:O	1:A:217:GLU:HB3	2.16	0.46
1:A:198:MSE:HE3	1:A:228:ALA:CB	2.47	0.45
1:B:23:THR:HG22	4:B:1001:HOH:O	2.16	0.45
1:G:198:MSE:HE3	1:G:245:PHE:HE2	1.81	0.45
1:C:64:ILE:HD13	1:C:91:LYS:HE3	1.98	0.45
1:E:106[B]:MSE:CE	1:E:106[B]:MSE:HB2	2.46	0.45
1:F:112:SER:O	1:F:116:GLN:HG3	2.17	0.44
1:B:271:LYS:HZ2	1:C:23:THR:HG21	1.78	0.44
1:C:198:MSE:CE	1:C:231:TYR:HB2	2.48	0.44
1:F:106[B]:MSE:HG2	1:F:124:TYR:CD2	2.53	0.43
1:E:106[B]:MSE:CE	1:E:106[B]:MSE:CB	2.96	0.43
1:F:213:CYS:O	1:F:217:GLU:HB3	2.18	0.43
1:C:255:ARG:N	1:C:256:PRO:CD	2.82	0.43
1:E:240:ASP:OD1	1:E:243:VAL:HG23	2.19	0.43
1:C:198:MSE:HE3	1:C:226:ILE:CG2	2.49	0.43
1:G:198:MSE:HE3	1:G:245:PHE:CE2	2.54	0.43
1:A:27:VAL:HG21	1:A:46:PHE:CZ	2.54	0.43
1:C:216[B]:MSE:HE2	1:D:235:PRO:HA	2.00	0.43
1:H:128:ASP:OD2	1:H:128:ASP:N	2.52	0.42
1:C:294:ALA:N	1:C:295:PRO:CD	2.82	0.42
1:D:213:CYS:O	1:D:217:GLU:HB3	2.19	0.42
1:E:198:MSE:HE2	1:E:226:ILE:CG2	2.48	0.42
1:F:108:PHE:CE1	1:F:126:TRP:HB3	2.54	0.42
1:E:262:LEU:HD11	1:E:266:LYS:HE3	2.01	0.42
1:H:40:TYR:N	1:H:41:PRO:CD	2.82	0.42
1:G:106[B]:MSE:HG2	1:G:124:TYR:HD2	1.85	0.42
1:B:106:MSE:HE1	1:B:136:ASN:O	2.20	0.42
1:G:125:ASP:OD1	4:G:923:HOH:O	2.22	0.42
1:G:156:LYS:NZ	4:G:723:HOH:O	2.53	0.42
1:A:213:CYS:O	1:A:218:MSE:HG3	2.20	0.42
1:D:211:SER:O	1:D:216[B]:MSE:HE3	2.20	0.42
1:E:106[B]:MSE:HA	1:E:122:ALA:O	2.20	0.42
1:B:27:VAL:HG23	1:B:53:ILE:HG21	2.01	0.42
1:D:106:MSE:HE2	1:D:106:MSE:HB3	1.97	0.42
1:E:156:LYS:HE3	1:E:288:SER:HB2	2.02	0.42
1:G:198:MSE:CE	1:G:245:PHE:HE2	2.33	0.42
1:F:30:VAL:O	1:F:79:LEU:HA	2.20	0.42
1:H:99:LYS:NZ	4:H:795:HOH:O	2.53	0.42
1:B:198:MSE:CE	1:B:231:TYR:HB2	2.50	0.41
1:F:198[B]:MSE:HE2	1:F:247:ILE:CD1	2.50	0.41
1:H:106[B]:MSE:CE	1:H:139:VAL:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:MSE:CE	1:B:226:ILE:CB	2.78	0.41
1:C:108:PHE:CE1	1:C:126:TRP:HB3	2.55	0.41
1:A:29:PHE:HB3	1:A:39:MSE:SE	2.70	0.41
1:E:194:ILE:HD12	1:F:194:ILE:HD12	2.01	0.41
1:D:106:MSE:HE3	1:D:139:VAL:HG11	2.03	0.41
1:F:23:THR:OG1	1:H:271:LYS:NZ	2.52	0.41
1:E:107:THR:O	1:E:123:GLN:HA	2.19	0.41
1:B:156:LYS:HE3	1:B:288:SER:HB2	2.03	0.41
1:C:324:TRP:O	1:G:109:LYS:NZ	2.53	0.41
1:F:217:GLU:OE2	1:F:323:MSE:HE1	2.21	0.41
1:C:34:GLY:O	1:C:38:ILE:HG23	2.20	0.41
1:A:40:TYR:N	1:A:41:PRO:CD	2.84	0.40
1:A:106:MSE:HE1	1:A:136:ASN:O	2.21	0.40
1:G:172[A]:GLU:OE2	4:G:1473:HOH:O	2.22	0.40
1:C:211:SER:O	1:C:216[A]:MSE:HG3	2.21	0.40
1:G:198:MSE:HG3	1:G:226:ILE:O	2.22	0.40
1:B:249:LEU:N	1:B:249:LEU:HD12	2.37	0.40
1:D:198[B]:MSE:HE3	1:D:261:ALA:HB1	2.02	0.40
1:E:27:VAL:HG23	1:E:53:ILE:HG21	2.04	0.40
1:C:106:MSE:HE1	1:C:136:ASN:O	2.21	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	325/329 (99%)	316 (97%)	9 (3%)	0	100	100
1	B	325/329 (99%)	318 (98%)	7 (2%)	0	100	100
1	C	325/329 (99%)	318 (98%)	7 (2%)	0	100	100
1	D	326/329 (99%)	319 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	325/329 (99%)	317 (98%)	8 (2%)	0	100	100
1	F	331/329 (101%)	323 (98%)	8 (2%)	0	100	100
1	G	329/329 (100%)	323 (98%)	6 (2%)	0	100	100
1	H	328/329 (100%)	323 (98%)	5 (2%)	0	100	100
All	All	2614/2632 (99%)	2557 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	266/267 (100%)	265 (100%)	1 (0%)	91	91
1	B	263/267 (98%)	261 (99%)	2 (1%)	81	82
1	C	267/267 (100%)	264 (99%)	3 (1%)	73	73
1	D	265/267 (99%)	263 (99%)	2 (1%)	81	82
1	E	265/267 (99%)	263 (99%)	2 (1%)	81	82
1	F	271/267 (102%)	270 (100%)	1 (0%)	91	91
1	G	270/267 (101%)	268 (99%)	2 (1%)	84	84
1	H	267/267 (100%)	266 (100%)	1 (0%)	91	91
All	All	2134/2136 (100%)	2120 (99%)	14 (1%)	86	84

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

Mol	Chain	Res	Type
1	A	236	PHE
1	B	236	PHE
1	B	303	ARG
1	C	236	PHE
1	C	323[A]	MSE
1	C	323[B]	MSE

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Mol	Chain	Res	Type
1	D	79	LEU
1	D	236	PHE
1	E	159	GLN
1	E	236	PHE
1	F	236	PHE
1	G	159	GLN
1	G	236	PHE
1	H	236	PHE

Sometimes 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 monosaccharides 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	FLC	C	329	-	12,12,12	1.27	1 (8%)	17,17,17	1.53	3 (17%)
3	GOL	H	330	-	5,5,5	0.57	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	H	329	-	12,12,12	1.20	1 (8%)	17,17,17	1.29	2 (11%)
3	GOL	C	330	-	5,5,5	0.46	0	5,5,5	0.89	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	FLC	C	329	-	-	2/16/16/16	-
3	GOL	H	330	-	-	3/4/4/4	-
2	FLC	H	329	-	-	0/16/16/16	-
3	GOL	C	330	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	329	FLC	CB-CBC	-2.74	1.50	1.53
2	C	329	FLC	CB-CBC	-2.24	1.51	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	329	FLC	OB1-CBC-CB	-3.21	117.70	122.25
2	H	329	FLC	OB1-CBC-CB	-2.67	118.47	122.25
2	C	329	FLC	OHB-CB-CBC	-2.65	105.14	108.86
2	C	329	FLC	OB2-CBC-CB	2.53	117.44	113.05
2	H	329	FLC	OB2-CBC-CB	2.20	116.88	113.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	330	GOL	C1-C2-C3-O3
3	C	330	GOL	C1-C2-C3-O3
3	H	330	GOL	O2-C2-C3-O3
3	C	330	GOL	O2-C2-C3-O3
2	C	329	FLC	OHB-CB-CG-CGC
3	C	330	GOL	O1-C1-C2-O2
3	H	330	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	329	FLC	CG-CB-CBC-OB2

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.31	1 (0%) 94 94	17, 22, 29, 36	0
1	B	318/329 (96%)	-0.23	2 (0%) 89 90	17, 22, 29, 36	0
1	C	318/329 (96%)	-0.29	2 (0%) 89 90	17, 22, 30, 38	0
1	D	318/329 (96%)	-0.20	2 (0%) 89 90	17, 22, 28, 37	0
1	E	318/329 (96%)	-0.36	1 (0%) 94 94	17, 22, 29, 37	0
1	F	322/329 (97%)	-0.36	2 (0%) 89 90	17, 22, 30, 38	0
1	G	321/329 (97%)	-0.29	0 100 100	17, 22, 30, 48	0
1	H	321/329 (97%)	-0.37	3 (0%) 84 85	17, 22, 30, 42	0
All	All	2555/2632 (97%)	-0.30	13 (0%) 91 92	17, 22, 30, 48	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	110	PRO	5.4
1	B	110	PRO	4.5
1	C	6	ALA	2.7
1	A	327	GLU	2.6
1	C	110	PRO	2.6
1	D	5	THR	2.6
1	H	110	PRO	2.5
1	B	6	ALA	2.4
1	E	324	TRP	2.3
1	F	111	GLU	2.3
1	D	284	ALA	2.2
1	H	111	GLU	2.1
1	H	128	ASP	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, 95th 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
3	GOL	C	330	6/6	0.80	0.19	41,46,47,49	0
2	FLC	H	329	13/13	0.81	0.17	35,40,44,46	0
2	FLC	C	329	13/13	0.81	0.16	38,42,44,47	0
3	GOL	H	330	6/6	0.86	0.28	37,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.