



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:27 AM GMT

PDB ID : 3O6X
Title : Crystal Structure of the type III Glutamine Synthetase from Bacteroides fragilis
Authors : van Rooyen, J.M.; Belrhali, H.; Abratt, V.R.; Sewell, B.T.
Deposited on : 2010-07-29
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

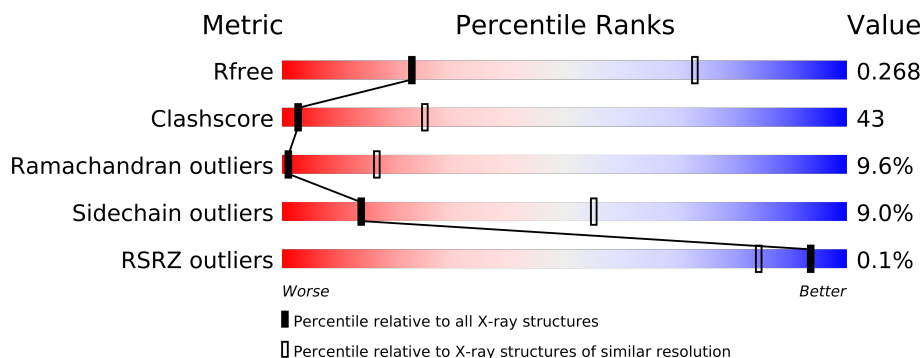
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	729	
1	B	729	
1	C	729	
1	D	729	
1	E	729	
1	F	729	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	C	2001	-	X
2	MG	D	2001	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	MG	F	2001	-	X
4	ADP	B	4001	-	X
4	ADP	E	4001	-	X
5	CL	B	5001	-	X
5	CL	C	5001	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30996 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	B	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	C	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	D	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	E	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			
1	F	638	Total	C	N	O	S	250	0	0
			5120	3253	889	948	30			

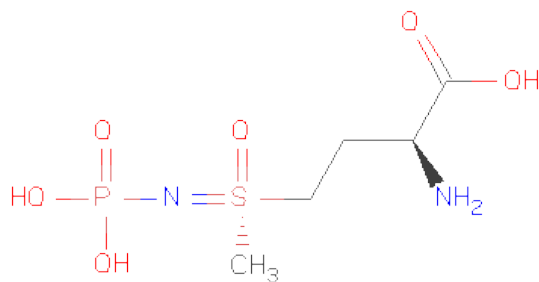
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLY	VAL	CONFLICT	UNP Q5LGP1
A	531	LEU	PRO	CONFLICT	UNP Q5LGP1
B	152	GLY	VAL	CONFLICT	UNP Q5LGP1
B	531	LEU	PRO	CONFLICT	UNP Q5LGP1
C	152	GLY	VAL	CONFLICT	UNP Q5LGP1
C	531	LEU	PRO	CONFLICT	UNP Q5LGP1
D	152	GLY	VAL	CONFLICT	UNP Q5LGP1
D	531	LEU	PRO	CONFLICT	UNP Q5LGP1
E	152	GLY	VAL	CONFLICT	UNP Q5LGP1
E	531	LEU	PRO	CONFLICT	UNP Q5LGP1
F	152	GLY	VAL	CONFLICT	UNP Q5LGP1
F	531	LEU	PRO	CONFLICT	UNP Q5LGP1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0

- Molecule 3 is L-METHIONINE-S-SULFOXIMINEPHOSPHATE (three-letter code: P3S) (formula: C₅H₁₃N₂O₆PS).



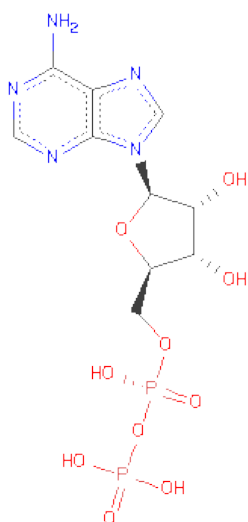
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 15 5 2 6 1 1	0	0
3	B	1	Total C N O P S 15 5 2 6 1 1	0	0
3	C	1	Total C N O P S 15 5 2 6 1 1	0	0
3	D	1	Total C N O P S 15 5 2 6 1 1	0	0
3	E	1	Total C N O P S 15 5 2 6 1 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
								0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	B	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	C	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	D	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	E	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	F	1	Total	C	N	O	P		
			27	10	5	10	2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Cl		
			2	2	0	0
5	E	2	Total	Cl		
			2	2	0	0

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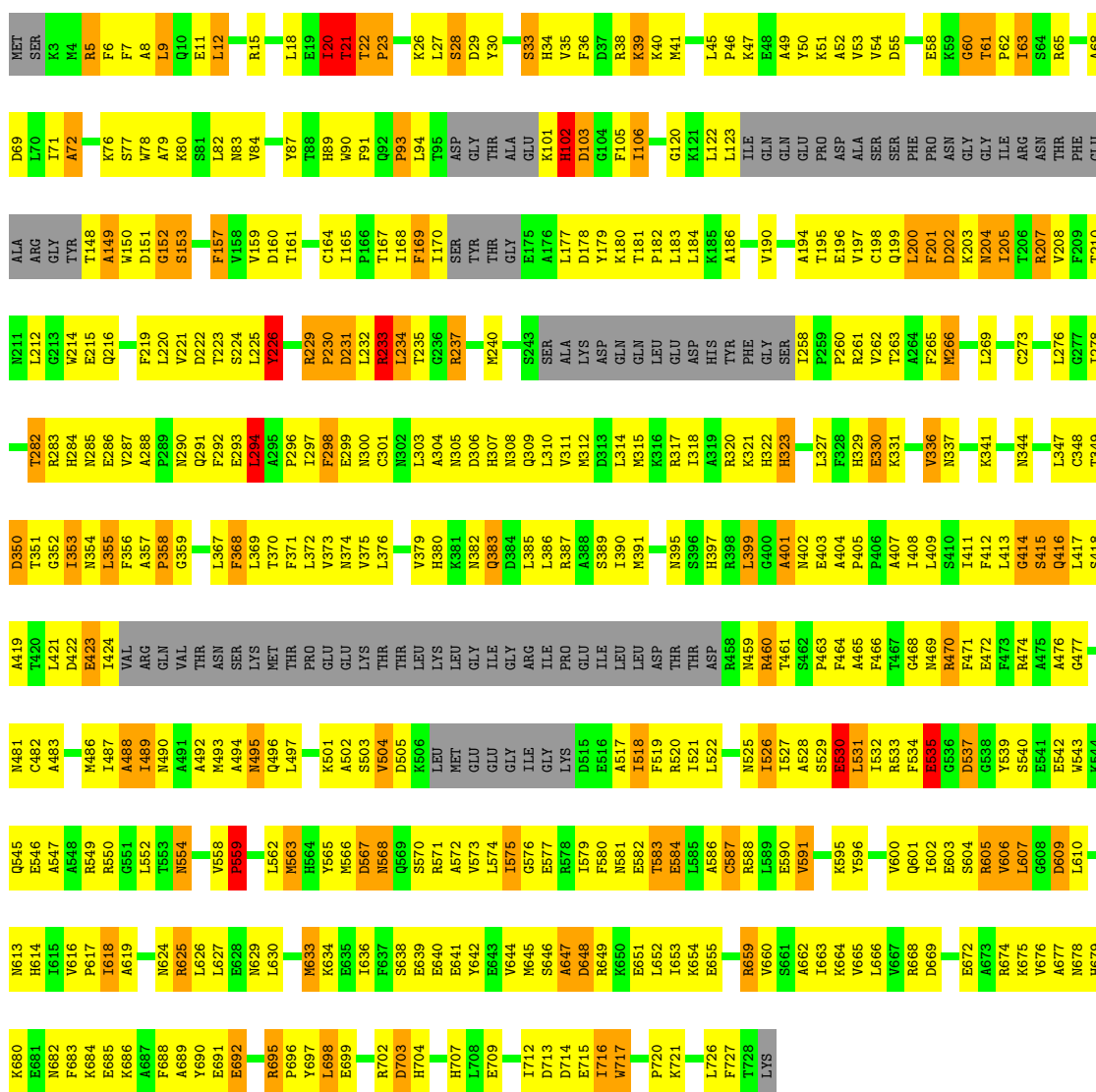
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Cl 2	0	0
5	C	2	Total 2	Cl 2	0	0
5	A	3	Total 3	Cl 3	0	0
5	F	1	Total 1	Cl 1	0	0

3 Residue-property plots

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.

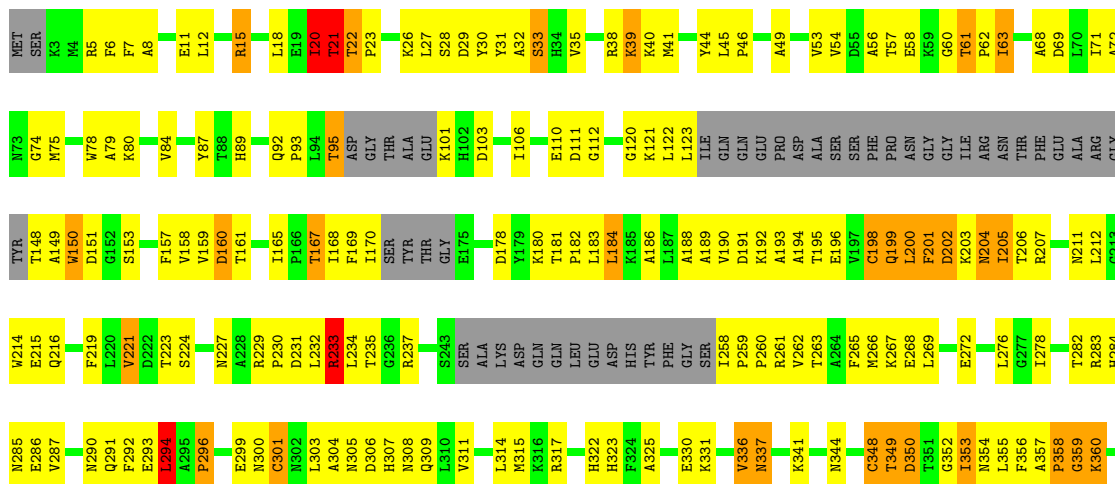
- Molecule 1: Glutamine synthetase

Chain A:



- Molecule 1: Glutamine synthetase

Chain B:

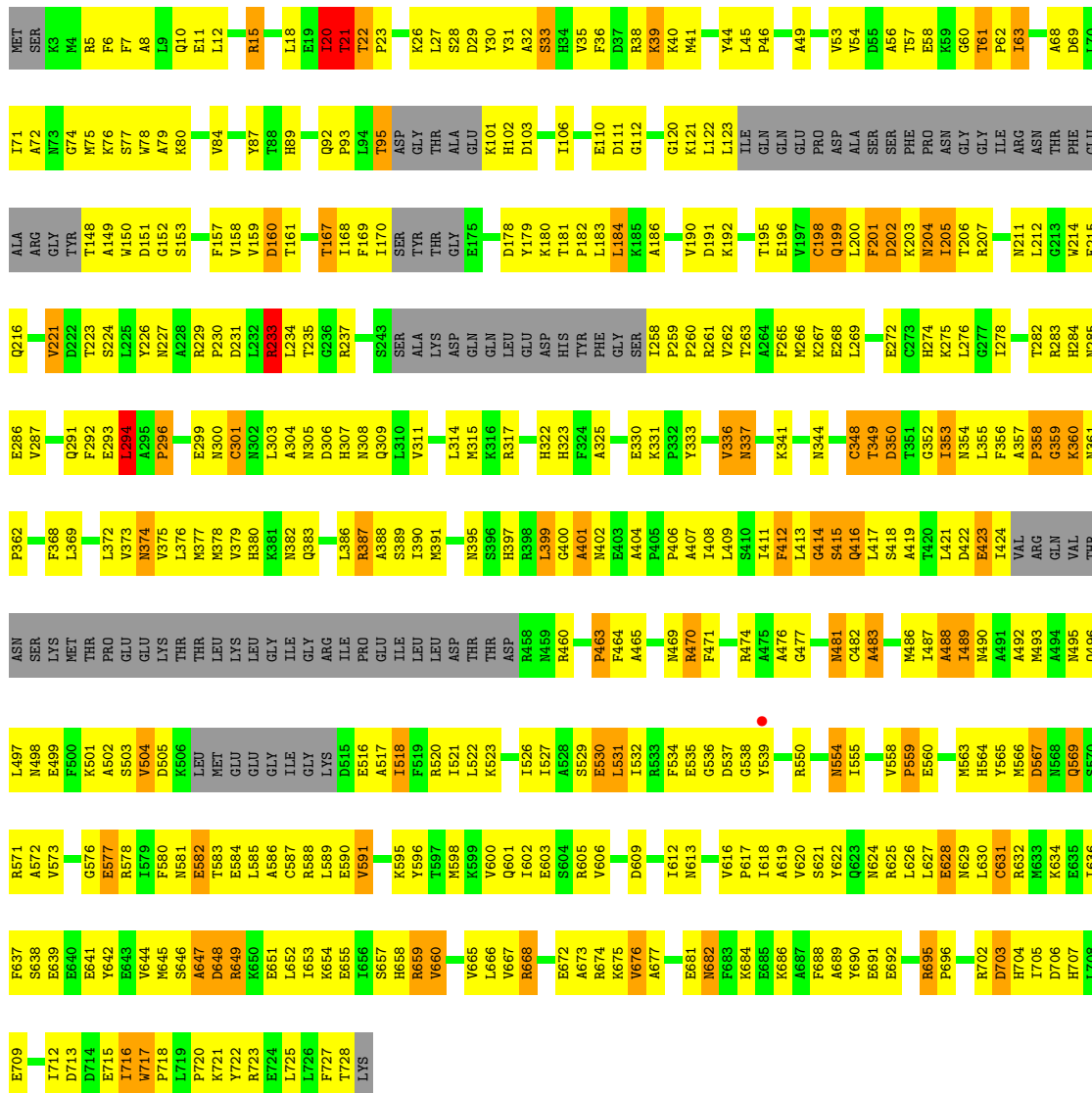






• Molecule 1: Glutamine synthetase

Chain E:



• Molecule 1: Glutamine synthetase

Chain F:



E715	E642	G576	E499	ASN	N361	H284	Q216
I716	E643	E577	F900	SER	P362	N285	F219
W717	V644	R578	K501	LYS	F368	E286	L220
P718	M645	R579	A502	THR	L369	V287	V221
L719	S646	I579	S503	PRO	N290	N290	D222
P720	A647	F580	V504	GLU	L372	Q291	T223
K721	D648	N581	D505	GLU	V373	F292	S224
Y722	R649	E582	K506	LYS	N374	E293	L225
R723	R650	T583	LEU	THR	V375	L294	Y226
E724	E651	E584	MET	THR	L376	A295	N227
L725	L652	L585	GLU	THR	L377	P296	A228
L726	I653	A586	GLU	LEU	N377	E299	R229
L727	K654	C587	GLY	LYS	N378	N300	P230
F727	E655	R588	ILE	LEU	V379	C301	D231
T728	I656	L589	GLY	GLY	H380	N302	L232
LYS	S657	E590	LYS	ILE	N381	L303	L234
	H658	V591	D515	ARG	Q382	A304	T235
	R659	E595	E516	ILE	Q383	N305	T236
	V660	Y596	A517	PRO	L386	D306	R237
		Y597	F519	GLU	R387	N307	
	T663	M598	R520	ILE	A388	N308	SER
	K664	K599	LEU	LEU	S389	Q309	ALA
	V665	V600	L522	ASP	T390	I310	LYS
	L666	Q601	K523	THR	N391	V311	ASP
	V667	I602		THR	N395	L314	GLN
	R668	E603	T626	ASP	S396	M315	GLN
	E672	S604	L527	ASP	R397	K316	LEU
	A673	R605	A528	R458	N398	R317	GLY
	R674	V606	S529	R459	L399		ASP
	K675	E609	E530	R460	G400		HIS
	V676	D609	L531	P463	A401		TYR
	A677	N613	L532	P464	N402		PHE
	E681	V616	F534	N469	E403		GLY
	N682	P617	E535	R470	A404		SER
	K686	I618	D537	F471	A407		T258
	A687	A619	G538		L408		F259
	F688	Y622	Y539	R474	L409		P260
	A689	Q623	R550	A475	S410		R261
	Y690	N624		A476	I411		V262
	E691	R625	N654	G477	F412		T263
	E692	L626	I555	M481	L413		K264
	P696	L627	V558	C482	G414		F265
		E628	V559	A483	Q416		M266
		N629			L417		K267
		L630		M486	S418		E268
	R702	G631	N563	I487	A419		L269
	D703	R632	H564	A488	T420		E272
	H704	F633	Y565	L421	L421		C273
	I705	K634	M566	N490	D422		H274
	D706	E635	D567	A491	E423		K275
	H707	L636	N568	A492	I424		L276
	L708	F637	Q569	M493	VAL		F277
	E709	S638	S570	Q496	ARG		I278
		E639	R571	GLN	P388		T282
	I712	E640	A572	VAL	G359		T283
	D713	V641		THR	N498		R283
	V714						

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	198.25Å 203.96Å 234.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.87 – 3.50 62.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.87-3.50) 100.0 (62.87-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.239 , 0.269 0.239 , 0.268	Depositor DCC
R_{free} test set	3016 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.3	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 60072 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	30996	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P3S, MG, ADP, CL

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	0.47	0/5223	0.68	1/7048 (0.0%)
1	B	0.43	0/5223	0.63	1/7048 (0.0%)
1	C	0.43	0/5223	0.63	1/7048 (0.0%)
1	D	0.43	0/5223	0.63	1/7048 (0.0%)
1	E	0.44	0/5223	0.63	1/7048 (0.0%)
1	F	0.43	0/5223	0.63	1/7048 (0.0%)
All	All	0.44	0/31338	0.64	6/42288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ARG	N-CA-C	-5.70	95.60	111.00
1	B	233	ARG	N-CA-C	-5.68	95.67	111.00
1	E	233	ARG	N-CA-C	-5.59	95.91	111.00
1	D	233	ARG	N-CA-C	-5.57	95.97	111.00
1	F	233	ARG	N-CA-C	-5.55	96.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	B	226	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5120	0	5090	481	0
1	B	5120	0	5090	415	1
1	C	5120	0	5090	402	0
1	D	5120	0	5090	406	0
1	E	5120	0	5090	415	0
1	F	5120	0	5090	409	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	15	0	10	1	0
3	B	15	0	10	0	0
3	C	15	0	10	0	0
3	D	15	0	10	0	0
3	E	15	0	10	0	0
3	F	15	0	10	0	0
4	A	27	0	12	4	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	2	0
4	F	27	0	12	2	0
5	A	3	0	0	5	0
5	B	2	0	0	4	0
5	C	2	0	0	4	0
5	D	2	0	0	4	0
5	E	2	0	0	4	0
5	F	1	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30996	0	30672	2496	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 43.

The worst 5 of 2496 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ILE:HD13	1:A:170:ILE:HD13	1.47	0.97
1:B:229:ARG:HD3	1:B:720:PRO:HD2	1.47	0.97
1:C:20:ILE:HG12	1:C:21:THR:H	1.31	0.96
1:F:229:ARG:HD3	1:F:720:PRO:HD2	1.46	0.96
1:F:20:ILE:HG12	1:F:21:THR:H	1.29	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:651:GLU:OE1	1:F:423:GLU:OE2[8_457]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	624/729 (86%)	408 (65%)	148 (24%)	68 (11%)	1	13
1	B	624/729 (86%)	438 (70%)	128 (20%)	58 (9%)	1	18
1	C	624/729 (86%)	441 (71%)	124 (20%)	59 (10%)	1	17
1	D	624/729 (86%)	433 (69%)	132 (21%)	59 (10%)	1	17
1	E	624/729 (86%)	444 (71%)	121 (19%)	59 (10%)	1	17
1	F	624/729 (86%)	442 (71%)	124 (20%)	58 (9%)	1	18
All	All	3744/4374 (86%)	2606 (70%)	777 (21%)	361 (10%)	1	17

5 of 361 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	23	PRO
1	A	149	ALA
1	A	204	ASN
1	A	234	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	554/631 (88%)	496 (90%)	58 (10%)	10	46
1	B	554/631 (88%)	506 (91%)	48 (9%)	15	57
1	C	554/631 (88%)	506 (91%)	48 (9%)	15	57
1	D	554/631 (88%)	505 (91%)	49 (9%)	14	57
1	E	554/631 (88%)	508 (92%)	46 (8%)	16	59
1	F	554/631 (88%)	505 (91%)	49 (9%)	14	57
All	All	3324/3786 (88%)	3026 (91%)	298 (9%)	14	55

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	387	ARG
1	D	184	LEU
1	F	350	ASP
1	C	481	ASN
1	C	676	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	678	ASN
1	D	382	ASN
1	F	481	ASN
1	C	707	HIS
1	D	285	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	P3S	A	3001	2	14,14,14	3.39	5 (35%)	19,21,21	3.93	7 (36%)
4	ADP	A	4001	2	29,29,29	1.11	2 (6%)	45,45,45	2.29	11 (24%)
3	P3S	B	3001	2	14,14,14	3.38	5 (35%)	19,21,21	4.03	7 (36%)
4	ADP	B	4001	2	29,29,29	1.11	2 (6%)	45,45,45	2.32	13 (28%)
3	P3S	C	3001	2	14,14,14	3.37	5 (35%)	19,21,21	4.03	7 (36%)
4	ADP	C	4001	2	29,29,29	1.11	2 (6%)	45,45,45	2.30	14 (31%)
3	P3S	D	3001	2	14,14,14	3.37	5 (35%)	19,21,21	4.03	7 (36%)
4	ADP	D	4001	2	29,29,29	1.11	2 (6%)	45,45,45	2.32	14 (31%)
3	P3S	E	3001	2	14,14,14	3.38	5 (35%)	19,21,21	4.04	7 (36%)
4	ADP	E	4001	2	29,29,29	1.10	2 (6%)	45,45,45	2.31	14 (31%)
3	P3S	F	3001	2	14,14,14	3.39	5 (35%)	19,21,21	4.05	7 (36%)
4	ADP	F	4001	2	29,29,29	1.11	2 (6%)	45,45,45	2.32	14 (31%)

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	P3S	A	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	A	4001	2	-	0/16/32/32	0/1/3/3
3	P3S	B	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	B	4001	2	-	0/16/32/32	0/1/3/3
3	P3S	C	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	C	4001	2	-	0/16/32/32	0/1/3/3
3	P3S	D	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	D	4001	2	-	0/16/32/32	0/1/3/3
3	P3S	E	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	E	4001	2	-	0/16/32/32	0/1/3/3
3	P3S	F	3001	2	-	1/13/16/16	0/0/0/0
4	ADP	F	4001	2	-	0/16/32/32	0/1/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3001	P3S	PA-O1A	9.11	1.61	1.46
3	E	3001	P3S	PA-O1A	9.09	1.61	1.46
3	F	3001	P3S	PA-O1A	9.09	1.61	1.46
3	D	3001	P3S	PA-O1A	9.07	1.61	1.46
3	C	3001	P3S	PA-O1A	9.06	1.61	1.46

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3001	P3S	OE-SD-CG	-12.01	99.70	108.21
3	D	3001	P3S	OE-SD-CG	-12.00	99.70	108.21
3	C	3001	P3S	OE-SD-CG	-11.86	99.80	108.21
3	E	3001	P3S	OE-SD-CG	-11.85	99.81	108.21
3	B	3001	P3S	OE-SD-CG	-11.83	99.83	108.21

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3001	P3S	CB-CG-SD-NE
3	C	3001	P3S	CB-CG-SD-NE
3	E	3001	P3S	CB-CG-SD-NE
3	D	3001	P3S	CB-CG-SD-NE
3	F	3001	P3S	CB-CG-SD-NE

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	637/729 (87%)	-0.21	0	100	100	2, 25, 71, 127	51 (8%)
1	B	637/729 (87%)	-0.17	0	100	100	2, 33, 89, 150	51 (8%)
1	C	637/729 (87%)	-0.11	1 (0%)	93	80	2, 31, 85, 149	51 (8%)
1	D	637/729 (87%)	-0.19	0	100	100	2, 29, 79, 148	51 (8%)
1	E	637/729 (87%)	-0.20	1 (0%)	93	80	2, 32, 82, 169	51 (8%)
1	F	637/729 (87%)	-0.15	1 (0%)	93	80	2, 31, 81, 129	51 (8%)
All	All	3822/4374 (87%)	-0.17	3 (0%)	93	84	2, 30, 82, 169	306 (8%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	200	LEU	2.7
1	C	549	ARG	2.3
1	E	539	TYR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	C	2001	1/1	0.24	4.92	33,33,33,33	0
2	MG	D	2001	1/1	0.24	4.19	32,32,32,32	0
5	CL	C	5001	1/1	0.25	3.97	1,1,1,1	0
5	CL	B	5001	1/1	0.24	3.46	1,1,1,1	0
4	ADP	B	4001	27/27	0.34	3.05	102,116,127,128	0
2	MG	F	2001	1/1	0.21	2.32	30,30,30,30	0
4	ADP	E	4001	27/27	0.26	2.08	99,113,123,125	0
4	ADP	A	4001	27/27	0.26	1.57	80,94,104,106	0
4	ADP	D	4001	27/27	0.28	1.33	93,107,117,118	0
3	P3S	D	3001	15/15	0.27	1.29	118,128,135,138	0
2	MG	E	2001	1/1	0.19	1.14	41,41,41,41	0
4	ADP	C	4001	27/27	0.22	1.12	99,113,124,125	0
4	ADP	F	4001	27/27	0.27	1.08	88,102,113,114	0
3	P3S	F	3001	15/15	0.29	1.00	118,128,135,138	0
3	P3S	A	3001	15/15	0.30	0.91	118,128,135,138	0
5	CL	A	730	1/1	0.20	0.89	1,1,1,1	0
3	P3S	E	3001	15/15	0.27	0.71	118,128,135,138	0
3	P3S	C	3001	15/15	0.24	0.47	118,128,135,138	0
5	CL	D	5001	1/1	0.19	0.47	1,1,1,1	0
3	P3S	B	3001	15/15	0.22	0.34	118,128,135,138	0
5	CL	A	5001	1/1	0.17	-0.04	1,1,1,1	0
5	CL	D	6001	1/1	0.16	-0.45	4,4,4,4	0
2	MG	A	1001	1/1	0.15	-0.67	3,3,3,3	0
5	CL	E	6001	1/1	0.13	-0.74	5,5,5,5	0
2	MG	B	2001	1/1	0.17	-0.76	52,52,52,52	0
2	MG	B	1001	1/1	0.15	-1.13	15,15,15,15	0
2	MG	D	1001	1/1	0.17	-1.17	10,10,10,10	0
5	CL	A	6001	1/1	0.12	-1.28	2,2,2,2	0
5	CL	E	5001	1/1	0.13	-1.68	1,1,1,1	0
5	CL	F	6001	1/1	0.13	-1.80	1,1,1,1	0
2	MG	C	1001	1/1	0.12	-1.91	8,8,8,8	0
5	CL	C	6001	1/1	0.09	-2.26	10,10,10,10	0
2	MG	A	2001	1/1	0.12	-2.50	37,37,37,37	0
2	MG	F	1001	1/1	0.11	-2.72	23,23,23,23	0
5	CL	B	6001	1/1	0.07	-3.09	5,5,5,5	0
2	MG	E	1001	1/1	0.06	-3.75	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.