Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:36 PM GMT

PDB ID	:	5DM3
Title	:	Crystal Structure of Glutamine Synthetase from Chromohalobacter salexigens DSM 3043(Csal_0679, TARGET EFI-550015) with bound ADP
Authors	:	Yadava, U.; Vetting, M.W.; Al Obaidi, N.F.; Toro, R.; Morisco, L.L.; Benach, J.; Koss, J.; Wasserman, S.R.; Attonito, J.D.; Scott Glenn, A.; Chamala, S.; Chowdhury, S.; Lafleur, J.; Love, J.; Seidel, R.D.; Whalen, K.L.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2015-09-07
Resolution	:	2.60 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:

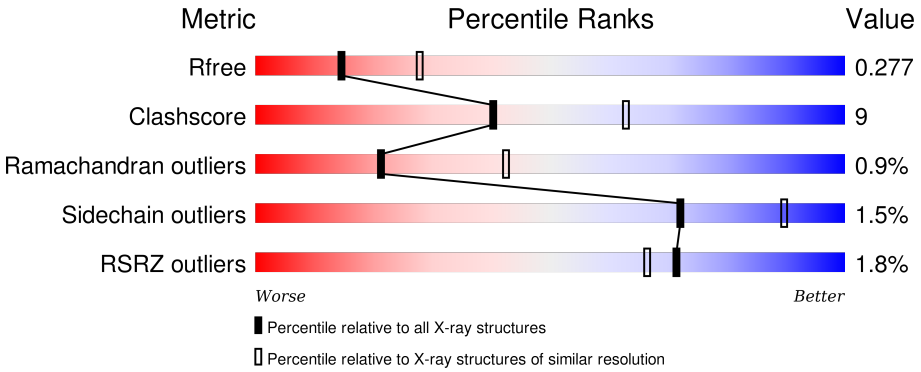
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	475	2% 63% 15% • 21%
1	B	475	% 60% 21% • 19%
1	C	475	% 67% 16% 17%
1	D	475	% 65% 16% • 19%
1	E	475	2% 63% 17% • 19%

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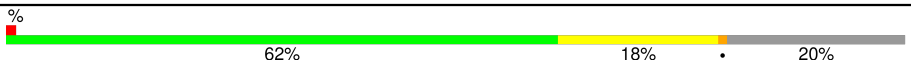
Mol	Chain	Length	Quality of chain
1	F	475	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17834 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 L-glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2859	1812	509	518	20			
1	B	385	Total	C	N	O	S	0	0	0
			2960	1871	525	543	21			
1	C	396	Total	C	N	O	S	0	1	0
			3014	1912	532	549	21			
1	D	386	Total	C	N	O	S	0	0	0
			2964	1876	527	540	21			
1	E	383	Total	C	N	O	S	0	0	0
			2925	1857	509	539	20			
1	F	381	Total	C	N	O	S	0	0	0
			2890	1837	507	525	21			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q1QZR8
A	-20	HIS	-	expression tag	UNP Q1QZR8
A	-19	HIS	-	expression tag	UNP Q1QZR8
A	-18	HIS	-	expression tag	UNP Q1QZR8
A	-17	HIS	-	expression tag	UNP Q1QZR8
A	-16	HIS	-	expression tag	UNP Q1QZR8
A	-15	HIS	-	expression tag	UNP Q1QZR8
A	-14	SER	-	expression tag	UNP Q1QZR8
A	-13	SER	-	expression tag	UNP Q1QZR8
A	-12	GLY	-	expression tag	UNP Q1QZR8
A	-11	VAL	-	expression tag	UNP Q1QZR8
A	-10	ASP	-	expression tag	UNP Q1QZR8
A	-9	LEU	-	expression tag	UNP Q1QZR8
A	-8	GLY	-	expression tag	UNP Q1QZR8
A	-7	THR	-	expression tag	UNP Q1QZR8
A	-6	GLU	-	expression tag	UNP Q1QZR8
A	-5	ASN	-	expression tag	UNP Q1QZR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP Q1QZR8
A	-3	TYR	-	expression tag	UNP Q1QZR8
A	-2	PHE	-	expression tag	UNP Q1QZR8
A	-1	GLN	-	expression tag	UNP Q1QZR8
A	0	SER	-	expression tag	UNP Q1QZR8
B	-21	MET	-	initiating methionine	UNP Q1QZR8
B	-20	HIS	-	expression tag	UNP Q1QZR8
B	-19	HIS	-	expression tag	UNP Q1QZR8
B	-18	HIS	-	expression tag	UNP Q1QZR8
B	-17	HIS	-	expression tag	UNP Q1QZR8
B	-16	HIS	-	expression tag	UNP Q1QZR8
B	-15	HIS	-	expression tag	UNP Q1QZR8
B	-14	SER	-	expression tag	UNP Q1QZR8
B	-13	SER	-	expression tag	UNP Q1QZR8
B	-12	GLY	-	expression tag	UNP Q1QZR8
B	-11	VAL	-	expression tag	UNP Q1QZR8
B	-10	ASP	-	expression tag	UNP Q1QZR8
B	-9	LEU	-	expression tag	UNP Q1QZR8
B	-8	GLY	-	expression tag	UNP Q1QZR8
B	-7	THR	-	expression tag	UNP Q1QZR8
B	-6	GLU	-	expression tag	UNP Q1QZR8
B	-5	ASN	-	expression tag	UNP Q1QZR8
B	-4	LEU	-	expression tag	UNP Q1QZR8
B	-3	TYR	-	expression tag	UNP Q1QZR8
B	-2	PHE	-	expression tag	UNP Q1QZR8
B	-1	GLN	-	expression tag	UNP Q1QZR8
B	0	SER	-	expression tag	UNP Q1QZR8
C	-21	MET	-	initiating methionine	UNP Q1QZR8
C	-20	HIS	-	expression tag	UNP Q1QZR8
C	-19	HIS	-	expression tag	UNP Q1QZR8
C	-18	HIS	-	expression tag	UNP Q1QZR8
C	-17	HIS	-	expression tag	UNP Q1QZR8
C	-16	HIS	-	expression tag	UNP Q1QZR8
C	-15	HIS	-	expression tag	UNP Q1QZR8
C	-14	SER	-	expression tag	UNP Q1QZR8
C	-13	SER	-	expression tag	UNP Q1QZR8
C	-12	GLY	-	expression tag	UNP Q1QZR8
C	-11	VAL	-	expression tag	UNP Q1QZR8
C	-10	ASP	-	expression tag	UNP Q1QZR8
C	-9	LEU	-	expression tag	UNP Q1QZR8
C	-8	GLY	-	expression tag	UNP Q1QZR8
C	-7	THR	-	expression tag	UNP Q1QZR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLU	-	expression tag	UNP Q1QZR8
C	-5	ASN	-	expression tag	UNP Q1QZR8
C	-4	LEU	-	expression tag	UNP Q1QZR8
C	-3	TYR	-	expression tag	UNP Q1QZR8
C	-2	PHE	-	expression tag	UNP Q1QZR8
C	-1	GLN	-	expression tag	UNP Q1QZR8
C	0	SER	-	expression tag	UNP Q1QZR8
D	-21	MET	-	initiating methionine	UNP Q1QZR8
D	-20	HIS	-	expression tag	UNP Q1QZR8
D	-19	HIS	-	expression tag	UNP Q1QZR8
D	-18	HIS	-	expression tag	UNP Q1QZR8
D	-17	HIS	-	expression tag	UNP Q1QZR8
D	-16	HIS	-	expression tag	UNP Q1QZR8
D	-15	HIS	-	expression tag	UNP Q1QZR8
D	-14	SER	-	expression tag	UNP Q1QZR8
D	-13	SER	-	expression tag	UNP Q1QZR8
D	-12	GLY	-	expression tag	UNP Q1QZR8
D	-11	VAL	-	expression tag	UNP Q1QZR8
D	-10	ASP	-	expression tag	UNP Q1QZR8
D	-9	LEU	-	expression tag	UNP Q1QZR8
D	-8	GLY	-	expression tag	UNP Q1QZR8
D	-7	THR	-	expression tag	UNP Q1QZR8
D	-6	GLU	-	expression tag	UNP Q1QZR8
D	-5	ASN	-	expression tag	UNP Q1QZR8
D	-4	LEU	-	expression tag	UNP Q1QZR8
D	-3	TYR	-	expression tag	UNP Q1QZR8
D	-2	PHE	-	expression tag	UNP Q1QZR8
D	-1	GLN	-	expression tag	UNP Q1QZR8
D	0	SER	-	expression tag	UNP Q1QZR8
E	-21	MET	-	initiating methionine	UNP Q1QZR8
E	-20	HIS	-	expression tag	UNP Q1QZR8
E	-19	HIS	-	expression tag	UNP Q1QZR8
E	-18	HIS	-	expression tag	UNP Q1QZR8
E	-17	HIS	-	expression tag	UNP Q1QZR8
E	-16	HIS	-	expression tag	UNP Q1QZR8
E	-15	HIS	-	expression tag	UNP Q1QZR8
E	-14	SER	-	expression tag	UNP Q1QZR8
E	-13	SER	-	expression tag	UNP Q1QZR8
E	-12	GLY	-	expression tag	UNP Q1QZR8
E	-11	VAL	-	expression tag	UNP Q1QZR8
E	-10	ASP	-	expression tag	UNP Q1QZR8
E	-9	LEU	-	expression tag	UNP Q1QZR8

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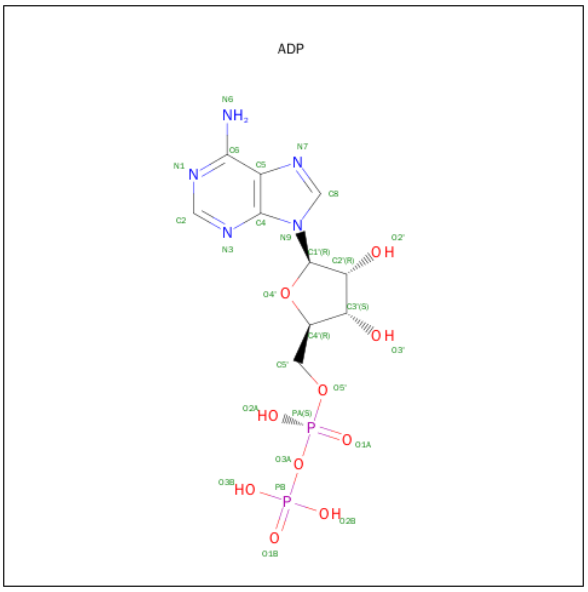
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	GLY	-	expression tag	UNP Q1QZR8
E	-7	THR	-	expression tag	UNP Q1QZR8
E	-6	GLU	-	expression tag	UNP Q1QZR8
E	-5	ASN	-	expression tag	UNP Q1QZR8
E	-4	LEU	-	expression tag	UNP Q1QZR8
E	-3	TYR	-	expression tag	UNP Q1QZR8
E	-2	PHE	-	expression tag	UNP Q1QZR8
E	-1	GLN	-	expression tag	UNP Q1QZR8
E	0	SER	-	expression tag	UNP Q1QZR8
F	-21	MET	-	initiating methionine	UNP Q1QZR8
F	-20	HIS	-	expression tag	UNP Q1QZR8
F	-19	HIS	-	expression tag	UNP Q1QZR8
F	-18	HIS	-	expression tag	UNP Q1QZR8
F	-17	HIS	-	expression tag	UNP Q1QZR8
F	-16	HIS	-	expression tag	UNP Q1QZR8
F	-15	HIS	-	expression tag	UNP Q1QZR8
F	-14	SER	-	expression tag	UNP Q1QZR8
F	-13	SER	-	expression tag	UNP Q1QZR8
F	-12	GLY	-	expression tag	UNP Q1QZR8
F	-11	VAL	-	expression tag	UNP Q1QZR8
F	-10	ASP	-	expression tag	UNP Q1QZR8
F	-9	LEU	-	expression tag	UNP Q1QZR8
F	-8	GLY	-	expression tag	UNP Q1QZR8
F	-7	THR	-	expression tag	UNP Q1QZR8
F	-6	GLU	-	expression tag	UNP Q1QZR8
F	-5	ASN	-	expression tag	UNP Q1QZR8
F	-4	LEU	-	expression tag	UNP Q1QZR8
F	-3	TYR	-	expression tag	UNP Q1QZR8
F	-2	PHE	-	expression tag	UNP Q1QZR8
F	-1	GLN	-	expression tag	UNP Q1QZR8
F	0	SER	-	expression tag	UNP Q1QZR8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is water.

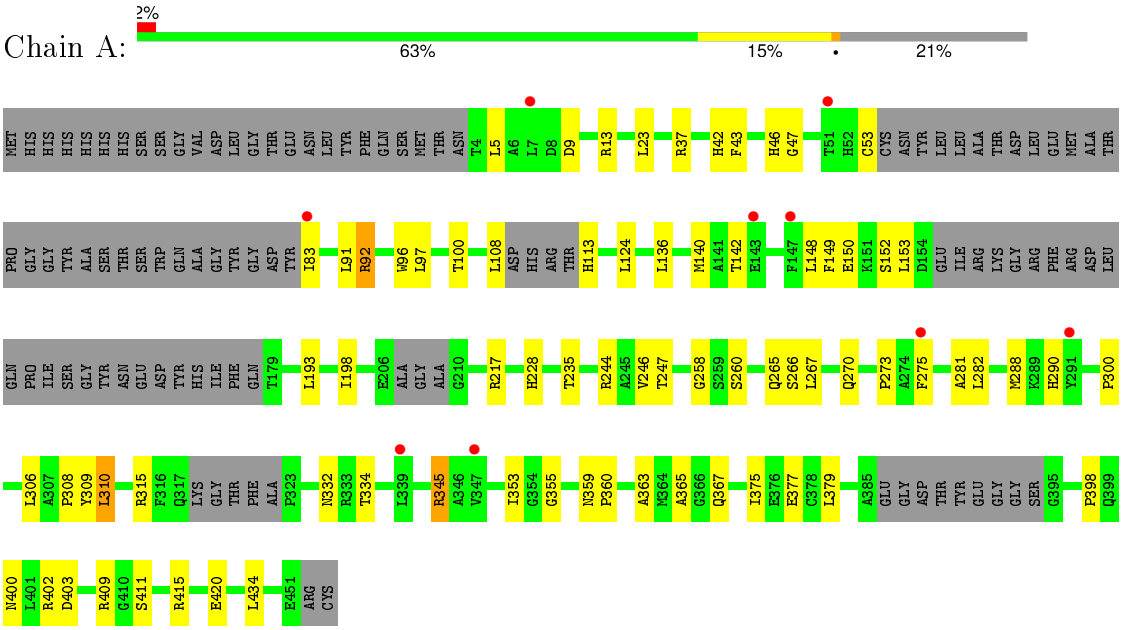
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	11	Total	O	0	0
			11	11		
3	C	11	Total	O	0	0
			11	11		
3	D	13	Total	O	0	0
			13	13		
3	E	7	Total	O	0	1
			8	8		
3	F	8	Total	O	0	0
			8	8		

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.

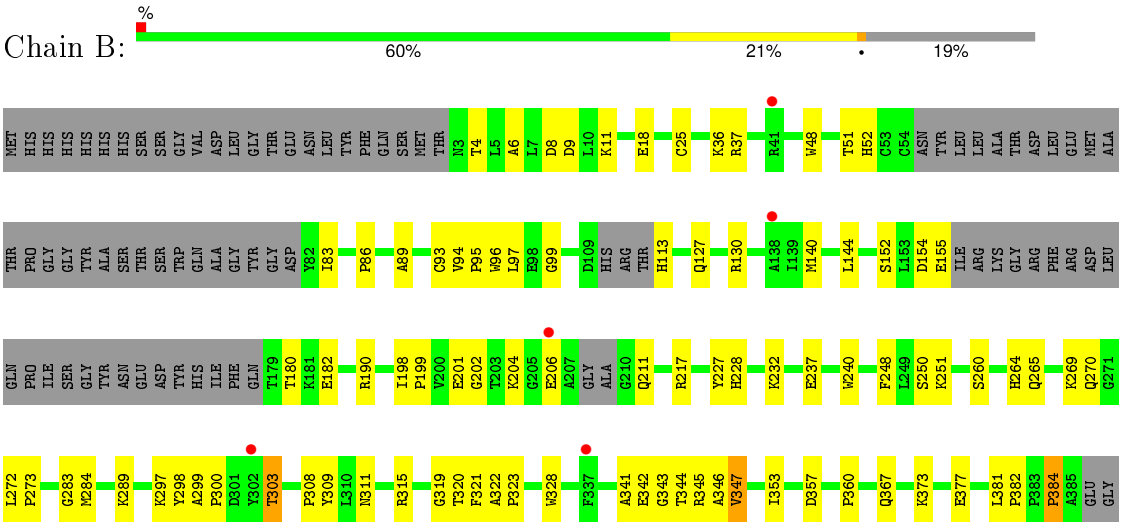
- Molecule 1: L-glutamine synthetase

Chain A:



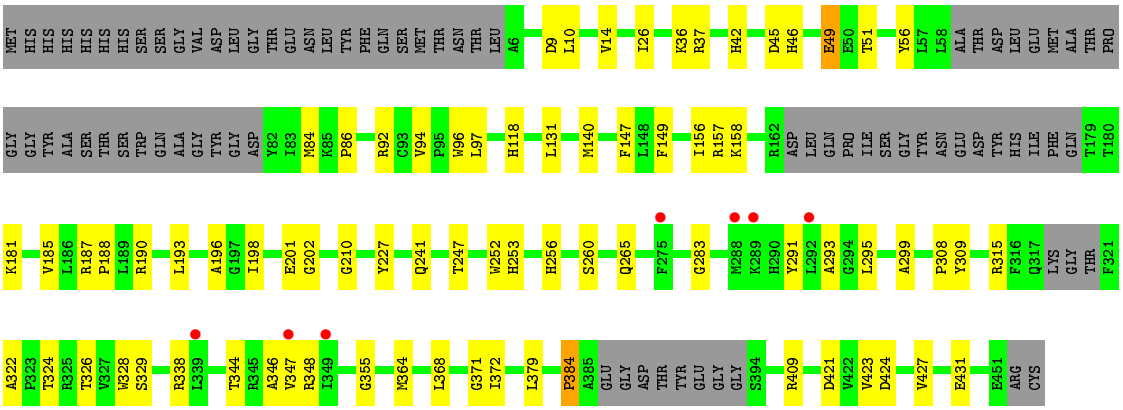
- Molecule 1: L-glutamine synthetase

Chain B:



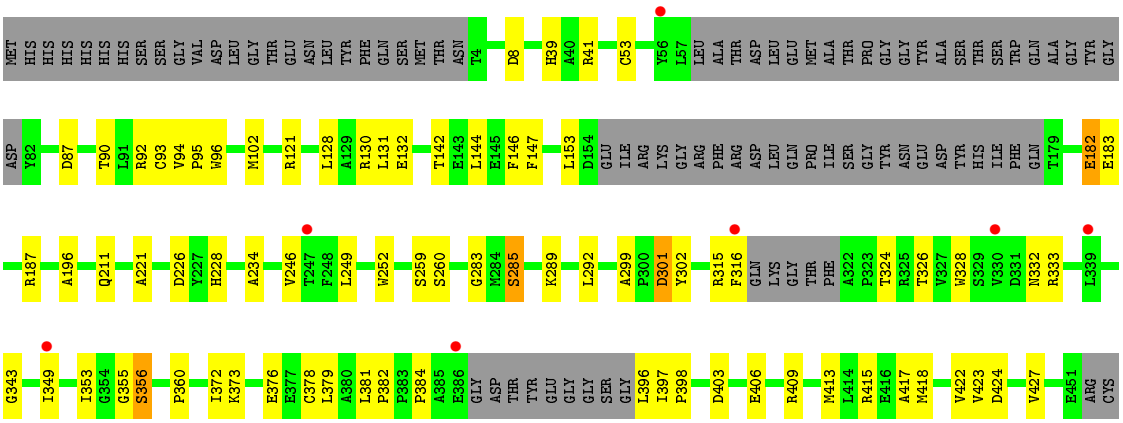
• Molecule 1: L-glutamine synthetase

Chain C:



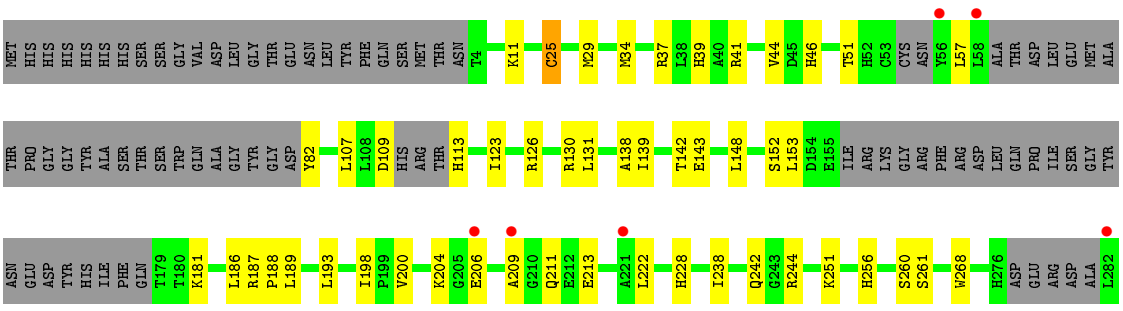
• Molecule 1: L-glutamine synthetase

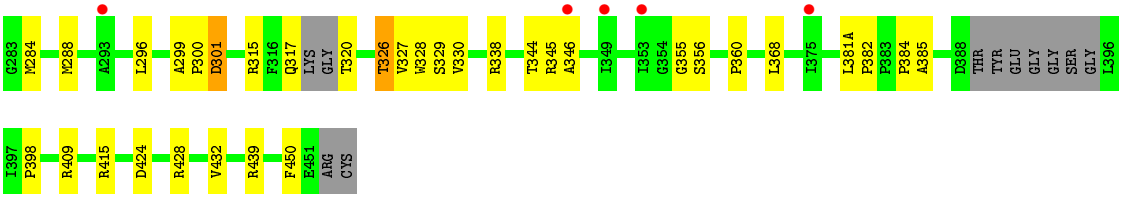
Chain D:



• Molecule 1: L-glutamine synthetase

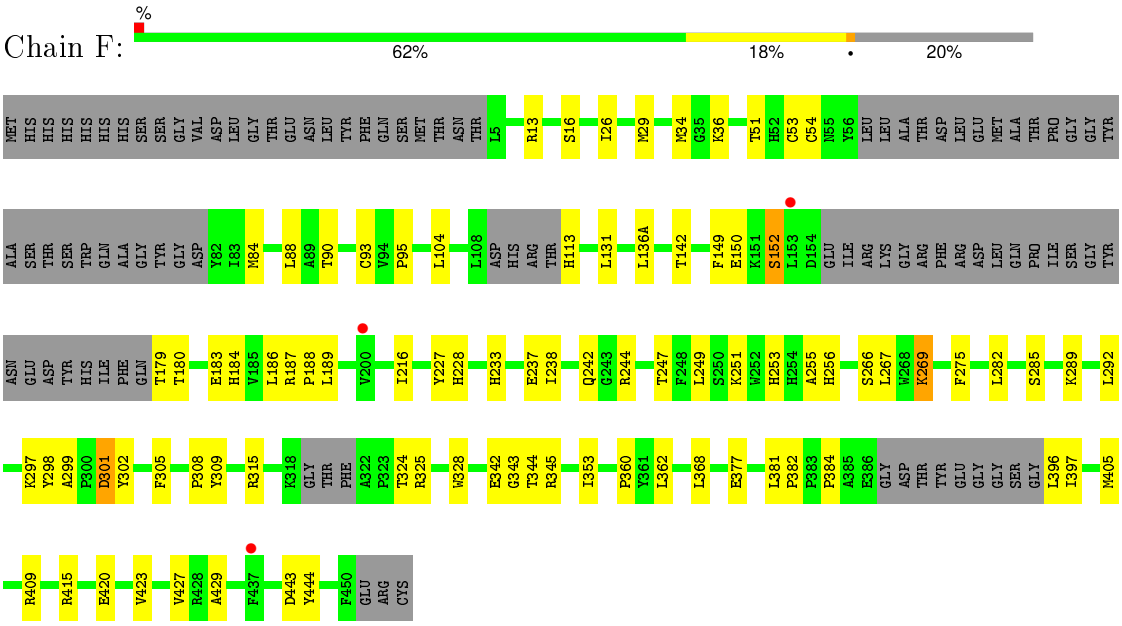
Chain E:





• Molecule 1: L-glutamine synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	132.98Å 221.34Å 199.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.06 – 2.60 113.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.06-2.60) 99.9 (113.99-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.274 0.218 , 0.277	Depositor DCC
R_{free} test set	4515 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.9	EDS
Estimated twinning fraction	0.027 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 90258 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17834	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: ADP

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	0.45	0/2918	0.59	0/3953
1	B	0.45	0/3022	0.62	0/4093
1	C	0.45	0/3080	0.61	0/4178
1	D	0.46	0/3026	0.59	0/4100
1	E	0.44	0/2984	0.60	0/4046
1	F	0.43	0/2951	0.59	0/4004
All	All	0.45	0/17981	0.60	0/24374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2859	0	2772	48	0
1	B	2960	0	2868	60	1
1	C	3014	0	2890	45	0
1	D	2964	0	2880	49	0
1	E	2925	0	2814	51	0
1	F	2890	0	2789	59	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
3	A	9	0	0	1	0
3	B	11	0	0	0	0
3	C	11	0	0	0	0
3	D	13	0	0	0	0
3	E	8	0	0	0	0
3	F	8	0	0	1	0
All	All	17834	0	17085	302	1

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

All (302) 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:A:142:THR:HG21	1:A:228:HIS:HD2	1.34	0.92
1:D:315:ARG:NH2	1:D:353:ILE:O	2.09	0.85
1:A:142:THR:HG21	1:A:228:HIS:CD2	2.12	0.85
1:E:415:ARG:NH2	1:E:424:ASP:OD1	2.13	0.81
1:C:51:THR:HB	1:C:84:MET:HB2	1.66	0.77
1:A:315:ARG:NH2	1:A:353:ILE:O	2.19	0.76
1:E:109:ASP:HB3	1:E:113:HIS:HA	1.69	0.75
1:E:330:VAL:O	1:E:338:ARG:NH1	2.19	0.74
1:D:142:THR:OG1	1:D:228:HIS:HD2	1.71	0.73
1:E:123:ILE:HG23	1:E:126:ARG:HH12	1.55	0.72
1:A:400:ASN:ND2	1:A:403:ASP:OD2	2.22	0.72
1:F:113:HIS:ND1	1:F:113:HIS:O	2.24	0.71
1:A:83:ILE:HG23	1:A:108:LEU:HB2	1.72	0.70
1:B:36:LYS:NZ	1:B:52:HIS:O	2.24	0.70
1:B:315:ARG:NH2	1:B:353:ILE:O	2.25	0.69
1:F:53:CYS:SG	1:F:54:CYS:N	2.65	0.69
1:A:150:GLU:H	1:A:150:GLU:CD	1.96	0.69
1:F:13:ARG:HA	1:F:16:SER:HB3	1.76	0.67
1:D:409:ARG:O	1:D:415:ARG:NH1	2.27	0.67
1:B:182:GLU:OE2	1:C:37:ARG:NH2	2.18	0.67
1:B:154:ASP:OD1	1:B:155:GLU:N	2.28	0.67
1:C:45:ASP:HB3	1:C:46[A]:HIS:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:MET:SD	1:F:409:ARG:NH1	2.68	0.66
1:D:182:GLU:OE1	1:E:37:ARG:NH1	2.27	0.66
1:B:373:LYS:HE3	1:B:377:GLU:OE2	1.95	0.66
1:B:269:LYS:O	1:B:272:LEU:HB2	1.96	0.66
1:D:144:LEU:HD13	1:D:228:HIS:NE2	2.11	0.65
1:D:283:GLY:HA3	1:D:343:GLY:HA2	1.79	0.65
1:F:247:THR:HG21	1:F:249:LEU:HD12	1.79	0.64
1:D:260:SER:HA	1:D:355:GLY:HA2	1.80	0.64
1:B:344:THR:O	1:B:347:VAL:HG23	1.97	0.63
1:F:228:HIS:ND1	1:F:360:PRO:HG3	2.13	0.63
1:E:139:ILE:HD12	1:E:268:TRP:CD1	2.34	0.62
1:A:260:SER:HA	1:A:355:GLY:HA2	1.81	0.62
1:E:123:ILE:HG23	1:E:126:ARG:NH1	2.15	0.62
1:F:131:LEU:HD11	1:F:368:LEU:HD22	1.80	0.62
1:C:36:LYS:HD2	1:C:51:THR:HG21	1.82	0.62
1:B:283:GLY:HA3	1:B:343:GLY:HA2	1.82	0.62
1:F:251:LYS:NZ	1:F:256:HIS:O	2.31	0.62
1:B:406:GLU:HA	1:B:409:ARG:HB3	1.81	0.62
1:D:249:LEU:HD23	1:D:252:TRP:HA	1.81	0.61
1:E:329:SER:OG	1:E:330:VAL:N	2.33	0.61
1:C:260:SER:HA	1:C:355:GLY:HA2	1.83	0.60
1:B:113:HIS:O	1:B:113:HIS:ND1	2.32	0.60
1:A:377:GLU:HB2	1:A:379:LEU:HG	1.83	0.60
1:E:260:SER:HA	1:E:355:GLY:HA2	1.84	0.59
1:B:206:GLU:HB2	1:B:211:GLN:HB3	1.83	0.59
1:D:228:HIS:ND1	1:D:360:PRO:HG3	2.17	0.58
1:D:373:LYS:HG3	1:D:413:MET:HG2	1.85	0.58
1:E:228:HIS:ND1	1:E:360:PRO:HG3	2.18	0.58
1:F:315:ARG:NH2	1:F:353:ILE:O	2.36	0.58
1:D:87:ASP:O	1:D:90:THR:OG1	2.15	0.58
1:F:149:PHE:HE2	1:F:247:THR:HG1	1.50	0.58
1:B:93:CYS:O	1:B:95:PRO:HD3	2.04	0.57
1:F:381:LEU:HD12	1:F:382:PRO:HD2	1.86	0.57
1:B:344:THR:HG22	1:B:346:ALA:H	1.70	0.56
1:D:328:TRP:CE2	1:D:384:PRO:HB3	2.41	0.56
1:A:96:TRP:O	1:A:97:LEU:HD12	2.04	0.56
1:F:247:THR:HG22	1:F:249:LEU:H	1.70	0.56
1:B:52:HIS:ND1	2:F:501:ADP:O1B	2.38	0.56
1:A:332:ASN:HD21	1:A:334:THR:HB	1.69	0.56
1:D:403:ASP:O	1:D:406:GLU:HG2	2.06	0.56
1:D:332:ASN:OD1	1:D:333:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:LEU:HD21	1:F:328:TRP:CG	2.42	0.55
1:B:8:ASP:HA	1:B:11:LYS:HB3	1.87	0.55
1:D:183:GLU:HG3	1:D:187:ARG:HB2	1.88	0.55
1:B:199:PRO:HB2	1:B:217:ARG:HB3	1.89	0.55
1:D:292:LEU:HD13	1:D:349:ILE:HG12	1.88	0.55
1:A:273:PRO:HG3	1:A:345:ARG:HD2	1.89	0.55
1:A:266:SER:HA	1:A:275:PHE:CE2	2.42	0.54
1:E:409:ARG:O	1:E:415:ARG:NH1	2.40	0.54
1:F:297:LYS:HD3	1:F:298:TYR:CZ	2.42	0.54
1:B:36:LYS:HZ3	1:B:51:THR:HG22	1.73	0.54
1:D:415:ARG:NH2	1:D:424:ASP:OD1	2.41	0.54
1:B:190:ARG:HD2	1:B:202:GLY:HA2	1.90	0.54
1:A:300:PRO:HB3	1:A:398:PRO:HD3	1.89	0.54
1:E:261:SER:HB2	1:E:356:SER:HA	1.89	0.53
1:A:308:PRO:HG2	1:A:309:TYR:CE2	2.42	0.53
1:A:402:ARG:HG3	1:A:434:LEU:HD22	1.91	0.53
1:A:113:HIS:O	1:A:113:HIS:ND1	2.42	0.53
1:C:328:TRP:CZ2	1:C:384:PRO:HG3	2.44	0.53
1:F:328:TRP:CZ2	1:F:384:PRO:HG3	2.44	0.53
1:A:306:LEU:HD13	1:A:353:ILE:HB	1.91	0.52
1:F:142:THR:OG1	1:F:228:HIS:HD2	1.91	0.52
1:B:228:HIS:ND1	1:B:360:PRO:HG3	2.25	0.52
1:C:140:MET:CE	1:C:265:GLN:HB3	2.40	0.52
1:A:124:LEU:HA	1:A:365:ALA:HB2	1.92	0.52
1:C:293:ALA:HB1	1:C:379:LEU:HG	1.92	0.52
1:E:284:MET:HG3	1:E:288:MET:SD	2.49	0.52
1:E:39:HIS:HE1	1:E:41:ARG:HG3	1.75	0.52
1:A:149:PHE:HE2	1:A:247:THR:HG22	1.75	0.52
1:D:316:PHE:HB3	1:D:324:THR:HG21	1.91	0.52
1:C:49:GLU:O	1:C:86:PRO:HD2	2.10	0.52
1:A:43:PHE:HA	1:A:47:GLY:HA3	1.91	0.52
1:E:327:VAL:HG21	1:E:385:ALA:HB3	1.92	0.52
1:E:328:TRP:CZ2	1:E:384:PRO:HG3	2.44	0.51
1:C:185:VAL:O	1:C:188:PRO:HD2	2.09	0.51
1:F:344:THR:HG22	1:F:345:ARG:H	1.76	0.51
1:A:9:ASP:O	1:A:13:ARG:HG2	2.10	0.51
1:F:415:ARG:HD3	1:F:420:GLU:OE1	2.11	0.51
1:C:326:THR:HG22	1:C:326:THR:O	2.10	0.51
1:B:198:ILE:HD12	1:B:227:TYR:CD1	2.46	0.51
1:C:94:VAL:HG11	1:C:97:LEU:HD12	1.92	0.50
1:D:259:SER:HB3	1:D:356:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:O	1:B:86:PRO:HG2	2.11	0.50
1:E:317:GLN:C	1:E:320:THR:HA	2.32	0.50
1:F:184:HIS:O	1:F:242:GLN:NE2	2.44	0.50
1:C:92:ARG:NH1	1:C:196:ALA:O	2.43	0.50
1:C:131:LEU:HB3	1:C:372:ILE:HD11	1.93	0.50
1:D:418:MET:HB3	1:D:422:VAL:HG21	1.94	0.50
1:B:37:ARG:HH12	1:F:186:LEU:HD12	1.75	0.50
1:F:305:PHE:CD1	1:F:362:LEU:HB3	2.47	0.49
1:B:284:MET:HE1	1:B:328:TRP:CH2	2.46	0.49
1:D:326:THR:HG22	1:D:396:LEU:N	2.27	0.49
1:E:142:THR:OG1	1:E:228:HIS:HD2	1.95	0.49
1:F:188:PRO:HG2	1:F:242:GLN:HE21	1.77	0.49
1:D:93:CYS:O	1:D:95:PRO:HD3	2.13	0.49
1:C:140:MET:HE2	1:C:265:GLN:HB3	1.95	0.49
1:E:204:LYS:HE2	1:F:36:LYS:HE2	1.95	0.49
1:A:363:ALA:O	1:A:367:GLN:HG3	2.12	0.49
1:B:18:GLU:O	1:B:99:GLY:HA2	2.12	0.49
1:B:6:ALA:HB3	1:B:9:ASP:HB2	1.95	0.49
1:C:140:MET:SD	1:C:364:MET:HE2	2.53	0.49
1:C:147:PHE:CE2	1:C:252:TRP:HD1	2.31	0.49
1:B:36:LYS:NZ	1:B:51:THR:HG22	2.29	0.48
1:B:328:TRP:CH2	1:B:384:PRO:HG3	2.48	0.48
1:B:201:GLU:HG2	1:C:42:HIS:CD2	2.49	0.48
1:B:144:LEU:HD21	1:B:232:LYS:HG3	1.96	0.48
1:F:325:ARG:HA	1:F:396:LEU:HD12	1.94	0.48
1:B:289:LYS:CB	1:B:381:LEU:HD11	2.44	0.48
1:A:228:HIS:ND1	1:A:360:PRO:HG3	2.29	0.48
1:A:148:LEU:HD22	1:A:244:ARG:HD2	1.95	0.48
1:E:143:GLU:HB3	1:E:213:GLU:OE2	2.13	0.48
1:E:152:SER:OG	1:E:153:LEU:N	2.47	0.48
1:C:253:HIS:HB3	1:C:256:HIS:ND1	2.29	0.47
1:C:322:ALA:O	1:C:324:THR:N	2.48	0.47
1:B:328:TRP:CZ2	1:B:384:PRO:HG3	2.50	0.47
1:A:152:SER:OG	1:A:153:LEU:N	2.48	0.47
1:D:299:ALA:HA	1:D:302:TYR:CE2	2.49	0.47
1:D:423:VAL:O	1:D:427:VAL:HG23	2.15	0.47
1:C:295:LEU:O	1:C:299:ALA:HB2	2.14	0.47
1:A:140:MET:CE	1:A:265:GLN:HB3	2.44	0.47
1:A:415:ARG:HD3	1:A:420:GLU:OE1	2.14	0.47
1:C:364:MET:O	1:C:368:LEU:HG	2.15	0.47
1:A:411:SER:O	1:A:415:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:HB3	1:A:375:ILE:HA	1.97	0.47
1:F:183:GLU:HG3	1:F:187:ARG:HB2	1.97	0.47
1:D:8:ASP:N	1:D:8:ASP:OD1	2.47	0.47
1:D:301:ASP:OD1	1:D:301:ASP:N	2.48	0.47
1:B:204:LYS:HB3	1:B:204:LYS:HE2	1.64	0.46
1:B:127:GLN:HA	1:B:130:ARG:HG3	1.96	0.46
1:F:443:ASP:OD1	1:F:444:TYR:N	2.48	0.46
1:F:324:THR:HG23	1:F:397:ILE:HG12	1.98	0.46
1:F:299:ALA:HA	1:F:302:TYR:CZ	2.50	0.46
1:F:93:CYS:O	1:F:95:PRO:HD3	2.15	0.46
1:C:26:ILE:HD11	1:C:56:TYR:CD2	2.51	0.46
1:A:359:ASN:HA	1:A:360:PRO:HD3	1.83	0.46
1:D:381:LEU:HD12	1:D:382:PRO:HD2	1.98	0.46
1:D:328:TRP:CZ2	1:D:384:PRO:HB3	2.50	0.46
1:B:180:THR:HG21	1:C:241:GLN:HE21	1.80	0.46
1:B:250:SER:OG	1:B:357:ASP:OD2	2.27	0.46
1:B:4:THR:HG21	1:B:89:ALA:O	2.14	0.46
1:B:52:HIS:CD2	1:B:83:ILE:HG13	2.51	0.46
1:E:344:THR:C	1:E:346:ALA:H	2.19	0.46
1:A:332:ASN:ND2	1:A:334:THR:HB	2.30	0.46
1:E:193:LEU:HD22	1:E:198:ILE:HG13	1.98	0.46
1:F:285:SER:O	1:F:289:LYS:HG3	2.16	0.45
1:C:329:SER:O	1:C:338:ARG:HA	2.16	0.45
1:A:275:PHE:HA	1:A:288:MET:HB2	1.97	0.45
1:E:198:ILE:O	1:E:200:VAL:HG23	2.16	0.45
1:E:381(A):LEU:HA	1:E:382:PRO:HD3	1.82	0.45
1:D:372:ILE:O	1:D:376:GLU:HG3	2.16	0.45
1:C:344:THR:C	1:C:346:ALA:H	2.20	0.45
1:D:397:ILE:HG12	1:D:398:PRO:HD2	1.98	0.45
1:F:150:GLU:O	1:F:244:ARG:NH1	2.48	0.45
1:F:29:MET:HE1	1:F:429:ALA:HB1	1.98	0.45
1:B:94:VAL:HG13	1:B:96:TRP:CE2	2.51	0.45
1:F:328:TRP:CH2	1:F:384:PRO:HG3	2.51	0.45
1:D:121:ARG:NH1	1:D:226:ASP:OD1	2.50	0.45
1:E:301:ASP:OD1	1:E:301:ASP:N	2.50	0.45
1:E:11:LYS:HE2	1:E:44:VAL:HB	1.98	0.45
1:B:94:VAL:HG13	1:B:96:TRP:CZ2	2.52	0.45
1:E:238:ILE:O	1:E:242:GLN:HG2	2.17	0.45
1:D:92:ARG:NH1	1:D:196:ALA:O	2.41	0.45
1:F:377:GLU:OE2	3:F:601:HOH:O	2.21	0.45
1:B:273:PRO:HG3	1:B:345:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD13	1:D:228:HIS:HE2	1.83	0.44
1:B:37:ARG:NH1	1:F:186:LEU:HD12	2.32	0.44
1:B:6:ALA:O	1:B:9:ASP:HB3	2.17	0.44
1:C:423:VAL:O	1:C:427:VAL:HG13	2.16	0.44
1:E:296:LEU:HD11	1:E:328:TRP:CD1	2.53	0.44
1:B:94:VAL:HG11	1:B:97:LEU:HD12	1.98	0.44
1:D:418:MET:HB3	1:D:422:VAL:CG2	2.48	0.44
1:F:216:ILE:HD13	1:F:227:TYR:HB3	2.00	0.44
1:B:299:ALA:HB3	1:B:300:PRO:HD3	1.99	0.44
1:A:92:ARG:NH2	3:A:601:HOH:O	2.48	0.44
1:C:283:GLY:O	1:C:347:VAL:HG21	2.18	0.44
1:A:23:LEU:CD2	1:A:37:ARG:HG2	2.48	0.44
1:A:409:ARG:HH21	1:A:409:ARG:HG3	1.83	0.44
1:E:25:CYS:HA	1:E:34:MET:O	2.17	0.44
1:F:53:CYS:HB2	1:F:84:MET:HG3	1.99	0.44
1:A:42:HIS:CD2	1:C:201:GLU:HG2	2.53	0.44
1:B:450:PHE:HA	1:B:451:GLU:C	2.38	0.44
1:E:148:LEU:HA	1:E:148:LEU:HD12	1.85	0.44
1:C:308:PRO:HG2	1:C:309:TYR:CE2	2.52	0.44
1:C:291:TYR:CE2	1:C:371:GLY:HA3	2.53	0.44
1:A:97:LEU:HD23	1:A:100:THR:HG21	2.00	0.44
1:F:189:LEU:HA	1:F:238:ILE:HD13	2.00	0.44
1:D:94:VAL:HG22	1:D:102:MET:HG2	2.00	0.44
1:A:258:GLY:HA3	1:A:315:ARG:HG3	2.00	0.44
1:D:131:LEU:HG	1:D:372:ILE:HD11	1.99	0.44
1:D:39:HIS:HE1	1:D:41:ARG:HG3	1.83	0.44
1:A:5:LEU:HD23	1:A:91:LEU:HG	2.00	0.44
1:B:308:PRO:HG2	1:B:309:TYR:CE2	2.52	0.44
1:F:342:GLU:HA	1:F:343:GLY:HA2	1.70	0.44
1:B:140:MET:HA	1:B:264:HIS:O	2.18	0.44
1:F:90:THR:HG21	1:F:104:LEU:HB2	1.99	0.43
1:E:82:TYR:HB3	1:E:107:LEU:HD11	2.00	0.43
1:E:39:HIS:CE1	1:E:41:ARG:HG3	2.52	0.43
1:C:348:ARG:HD2	2:C:501:ADP:C2	2.53	0.43
1:E:206:GLU:HG3	1:E:211:GLN:HG2	2.00	0.43
1:B:297:LYS:HE3	1:B:298:TYR:OH	2.18	0.43
1:B:341:ALA:O	1:B:344:THR:HB	2.18	0.43
1:E:222:LEU:HD12	1:E:222:LEU:HA	1.85	0.43
1:C:260:SER:HB3	1:C:315:ARG:NH1	2.34	0.43
1:A:308:PRO:HG2	1:A:309:TYR:CD2	2.53	0.43
1:C:156:ILE:C	1:C:158:LYS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:ARG:HG2	1:E:439:ARG:O	2.19	0.43
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.79	0.43
1:C:190:ARG:HD2	1:C:202:GLY:HA2	2.01	0.43
1:E:131:LEU:CD1	1:E:138:ALA:HB2	2.48	0.43
1:F:26:ILE:HG23	1:F:84:MET:HE2	1.99	0.43
1:F:36:LYS:HD2	1:F:51:THR:HG21	2.01	0.43
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.87	0.43
1:F:238:ILE:O	1:F:242:GLN:HG2	2.18	0.43
1:C:198:ILE:HG13	1:C:227:TYR:CD1	2.54	0.43
1:D:142:THR:OG1	1:D:228:HIS:CD2	2.61	0.43
1:B:381:LEU:HA	1:B:382:PRO:HD2	1.88	0.43
1:D:130:ARG:HH12	1:D:417:ALA:CB	2.32	0.43
1:E:300:PRO:HB3	1:E:398:PRO:HD3	2.01	0.43
1:F:266:SER:HA	1:F:275:PHE:CE2	2.54	0.43
1:D:285:SER:O	1:D:289:LYS:HG3	2.19	0.42
1:C:187:ARG:HB3	1:C:188:PRO:HD3	2.01	0.42
1:F:299:ALA:HA	1:F:302:TYR:CE2	2.55	0.42
1:E:189:LEU:HA	1:E:238:ILE:HD12	2.00	0.42
1:C:149:PHE:HE2	1:C:247:THR:HG22	1.84	0.42
1:A:217:ARG:HB3	1:A:217:ARG:HE	1.58	0.42
1:D:299:ALA:HA	1:D:302:TYR:CZ	2.55	0.42
1:C:424:ASP:O	1:C:427:VAL:HG22	2.20	0.42
1:F:152:SER:OG	1:F:152:SER:O	2.37	0.42
1:B:240:TRP:CZ3	1:F:180:THR:HB	2.54	0.42
1:D:96:TRP:CZ2	1:D:234:ALA:HB2	2.54	0.42
1:D:147:PHE:CE1	1:D:211:GLN:HB2	2.55	0.42
1:B:265:GLN:NE2	1:B:367:GLN:OE1	2.53	0.42
1:F:308:PRO:HG2	1:F:309:TYR:CE2	2.54	0.42
1:A:235:THR:HG22	1:A:246:VAL:HG11	2.02	0.42
1:D:353:ILE:HD13	1:D:397:ILE:CD1	2.50	0.42
1:D:131:LEU:HA	1:D:131:LEU:HD23	1.83	0.42
1:B:251:LYS:O	1:B:311:ASN:ND2	2.44	0.42
1:F:233:HIS:O	1:F:237:GLU:HG2	2.20	0.42
1:F:136(A):LEU:HD13	1:F:267:LEU:HD13	2.02	0.42
1:F:301:ASP:OD1	1:F:301:ASP:N	2.52	0.42
1:F:188:PRO:HG2	1:F:242:GLN:NE2	2.35	0.42
1:B:342:GLU:N	1:B:342:GLU:OE2	2.40	0.42
1:C:409:ARG:NH2	1:C:431:GLU:OE2	2.53	0.41
1:D:260:SER:HB3	1:D:315:ARG:NH1	2.35	0.41
1:E:187:ARG:HB3	1:E:188:PRO:HD3	2.02	0.41
1:E:368:LEU:HA	1:E:368:LEU:HD23	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:VAL:HG13	1:C:96:TRP:CZ2	2.55	0.41
1:C:348:ARG:HH21	2:C:501:ADP:H5'1	1.86	0.41
1:B:232:LYS:HE3	1:B:248:PHE:CG	2.55	0.41
1:E:299:ALA:HB3	1:E:300:PRO:HD3	2.02	0.41
1:B:320:THR:O	1:B:322:ALA:N	2.50	0.41
1:F:53:CYS:HG	1:F:54:CYS:H	1.66	0.41
1:E:296:LEU:HD11	1:E:328:TRP:HD1	1.85	0.41
1:A:281:ALA:C	1:A:282:LEU:HD23	2.41	0.41
1:D:146:PHE:HD2	1:D:246:VAL:HG23	1.84	0.41
1:A:193:LEU:HD22	1:A:198:ILE:HD12	2.03	0.41
1:E:244:ARG:HD3	1:E:244:ARG:HA	1.93	0.41
1:E:260:SER:HB3	1:E:315:ARG:NH1	2.36	0.41
1:E:11:LYS:HB2	1:E:11:LYS:HE3	1.69	0.41
1:C:118:HIS:CD2	1:C:118:HIS:H	2.37	0.41
1:F:149:PHE:HE2	1:F:247:THR:OG1	2.04	0.41
1:A:149:PHE:HE2	1:A:247:THR:CG2	2.34	0.41
1:D:379:LEU:HA	1:D:379:LEU:HD23	1.83	0.41
1:F:253:HIS:CE1	1:F:255:ALA:H	2.39	0.41
1:B:237:GLU:OE1	1:F:179:THR:HB	2.20	0.41
1:A:149:PHE:O	1:A:244:ARG:HD3	2.20	0.41
1:D:128:LEU:O	1:D:132:GLU:HG3	2.21	0.41
1:E:428:ARG:O	1:E:432:VAL:HG12	2.21	0.41
1:F:269:LYS:HB2	1:F:269:LYS:HE2	1.84	0.41
1:B:405:MET:SD	1:B:431:GLU:HG3	2.61	0.41
1:E:126:ARG:O	1:E:130:ARG:HG3	2.20	0.40
1:C:10:LEU:O	1:C:14:VAL:HG23	2.21	0.40
1:E:251:LYS:HE3	1:E:256:HIS:O	2.22	0.40
1:F:423:VAL:O	1:F:427:VAL:HG23	2.21	0.40
1:E:29:MET:HG3	1:E:57:LEU:CD2	2.51	0.40
1:B:423:VAL:O	1:B:427:VAL:HG23	2.21	0.40
1:A:136:LEU:HD13	1:A:267:LEU:HD13	2.04	0.40
1:E:186:LEU:HD23	1:E:186:LEU:HA	1.79	0.40
1:F:88:LEU:HD22	1:F:88:LEU:H	1.85	0.40
1:B:303:THR:HG21	1:B:398:PRO:HD2	2.03	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASP:OD2	1:B:444:TYR:OH[3_555]	2.19	0.01

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	360/475 (76%)	348 (97%)	10 (3%)	2 (1%)	30	56
1	B	373/475 (78%)	352 (94%)	16 (4%)	5 (1%)	15	30
1	C	387/475 (82%)	360 (93%)	22 (6%)	5 (1%)	15	30
1	D	376/475 (79%)	358 (95%)	15 (4%)	3 (1%)	24	46
1	E	367/475 (77%)	339 (92%)	22 (6%)	6 (2%)	12	24
1	F	369/475 (78%)	351 (95%)	18 (5%)	0	100	100
All	All	2232/2850 (78%)	2108 (94%)	103 (5%)	21 (1%)	21	42

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	GLU
1	A	270	GLN
1	B	319	GLY
1	B	321	PHE
1	B	384	PRO
1	E	181	LYS
1	E	209	ALA
1	B	323	PRO
1	C	210	GLY
1	C	157	ARG
1	C	384	PRO
1	D	153	LEU
1	D	221	ALA
1	E	450	PHE
1	C	181	LYS
1	D	356	SER
1	A	46	HIS
1	B	347	VAL
1	E	46	HIS
1	E	326	THR

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Mol	Chain	Res	Type
1	E	345	ARG

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	285/386 (74%)	281 (99%)	4 (1%)	74	90
1	B	298/386 (77%)	292 (98%)	6 (2%)	63	85
1	C	297/386 (77%)	295 (99%)	2 (1%)	88	96
1	D	296/386 (77%)	291 (98%)	5 (2%)	68	88
1	E	291/386 (75%)	287 (99%)	4 (1%)	74	90
1	F	285/386 (74%)	280 (98%)	5 (2%)	66	87
All	All	1752/2316 (76%)	1726 (98%)	26 (2%)	72	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	92	ARG
1	A	310	LEU
1	A	345	ARG
1	B	25	CYS
1	B	152	SER
1	B	260	SER
1	B	270	GLN
1	B	303	THR
1	B	442	SER
1	C	9	ASP
1	C	421	ASP
1	D	53	CYS
1	D	182	GLU
1	D	285	SER
1	D	301	ASP
1	D	378	CYS

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Mol	Chain	Res	Type
1	E	25	CYS
1	E	51	THR
1	E	301	ASP
1	E	326	THR
1	F	34	MET
1	F	152	SER
1	F	269	LYS
1	F	282	LEU
1	F	301	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	B	3	ASN
1	D	228	HIS
1	E	228	HIS
1	F	184	HIS
1	F	228	HIS
1	F	242	GLN
1	F	265	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	ADP	A	501	-	24,29,29	0.95	1 (4%)	23,45,45	2.06	4 (17%)
2	ADP	B	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.97	2 (8%)
2	ADP	C	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.85	3 (13%)
2	ADP	D	501	-	24,29,29	0.92	1 (4%)	23,45,45	1.95	4 (17%)
2	ADP	E	501	-	24,29,29	0.99	1 (4%)	23,45,45	1.74	2 (8%)
2	ADP	F	501	-	24,29,29	0.98	1 (4%)	23,45,45	1.92	3 (13%)

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	ADP	A	501	-	-	0/12/32/32	0/3/3/3
2	ADP	B	501	-	-	0/12/32/32	0/3/3/3
2	ADP	C	501	-	-	0/12/32/32	0/3/3/3
2	ADP	D	501	-	-	0/12/32/32	0/3/3/3
2	ADP	E	501	-	-	0/12/32/32	0/3/3/3
2	ADP	F	501	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ADP	C5-C4	2.90	1.47	1.40
2	E	501	ADP	C5-C4	3.00	1.47	1.40
2	B	501	ADP	C5-C4	3.00	1.47	1.40
2	F	501	ADP	C5-C4	3.04	1.47	1.40
2	A	501	ADP	C5-C4	3.17	1.47	1.40
2	C	501	ADP	C5-C4	3.29	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	ADP	N3-C2-N1	-8.03	122.57	128.87
2	B	501	ADP	N3-C2-N1	-7.38	123.08	128.87
2	C	501	ADP	N3-C2-N1	-7.09	123.31	128.87
2	F	501	ADP	N3-C2-N1	-6.93	123.42	128.87
2	D	501	ADP	N3-C2-N1	-6.58	123.70	128.87
2	E	501	ADP	N3-C2-N1	-6.55	123.73	128.87
2	D	501	ADP	C4'-O4'-C1'	-2.76	106.72	109.64
2	A	501	ADP	C1'-N9-C4	-2.68	123.81	126.81
2	D	501	ADP	C1'-N9-C4	-2.29	124.24	126.81
2	F	501	ADP	O3B-PB-O2B	2.00	114.79	107.44
2	A	501	ADP	O3B-PB-O2B	2.02	114.86	107.44
2	C	501	ADP	N6-C6-N1	2.11	122.05	118.52
2	C	501	ADP	O4'-C1'-N9	2.26	112.37	108.11
2	E	501	ADP	O4'-C1'-N9	2.45	112.73	108.11
2	A	501	ADP	O4'-C1'-N9	2.66	113.13	108.11
2	B	501	ADP	O4'-C1'-N9	2.83	113.45	108.11
2	F	501	ADP	O4'-C1'-N9	3.37	114.47	108.11
2	D	501	ADP	O4'-C1'-N9	3.53	114.77	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ADP	2	0
2	F	501	ADP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	374/475 (78%)	0.08	9 (2%)	62	56	35, 58, 91, 127	0
1	B	385/475 (81%)	0.08	5 (1%)	79	75	36, 58, 92, 119	0
1	C	396/475 (83%)	0.04	7 (1%)	71	66	33, 55, 95, 133	0
1	D	386/475 (81%)	0.04	7 (1%)	71	66	32, 53, 87, 126	0
1	E	383/475 (80%)	0.05	11 (2%)	55	48	36, 60, 96, 148	0
1	F	381/475 (80%)	0.02	3 (0%)	87	85	37, 57, 90, 116	0
All	All	2305/2850 (80%)	0.05	42 (1%)	71	66	32, 56, 93, 148	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	GLU	7.7
1	A	51	THR	3.1
1	C	349	ILE	3.1
1	A	291	TYR	2.9
1	D	349	ILE	2.8
1	E	56	TYR	2.8
1	E	206	GLU	2.7
1	B	206	GLU	2.7
1	C	275	PHE	2.6
1	E	293	ALA	2.6
1	D	339	LEU	2.5
1	C	292	LEU	2.5
1	F	153	LEU	2.5
1	A	347	VAL	2.5
1	A	143	GLU	2.4
1	D	330	VAL	2.4
1	D	247	THR	2.4
1	E	375	ILE	2.3
1	C	339	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	209	ALA	2.3
1	B	302	TYR	2.3
1	D	56	TYR	2.3
1	A	339	LEU	2.3
1	B	337	PHE	2.3
1	F	437	PHE	2.3
1	B	138	ALA	2.2
1	C	288	MET	2.2
1	C	289	LYS	2.2
1	A	7	LEU	2.2
1	E	349	ILE	2.2
1	E	58	LEU	2.2
1	E	282	LEU	2.2
1	E	221	ALA	2.1
1	F	200	VAL	2.1
1	D	316	PHE	2.1
1	A	83	ILE	2.1
1	E	346	ALA	2.1
1	A	275	PHE	2.0
1	E	353	ILE	2.0
1	B	41	ARG	2.0
1	A	147	PHE	2.0
1	C	347	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	F	501	27/27	0.87	0.25	1.65	69,81,154,172	0
2	ADP	E	501	27/27	0.91	0.23	0.58	66,77,127,141	0
2	ADP	D	501	27/27	0.89	0.22	0.46	54,76,182,184	0
2	ADP	C	501	27/27	0.85	0.21	0.34	71,85,167,189	0
2	ADP	B	501	27/27	0.92	0.19	-0.05	45,61,141,142	0
2	ADP	A	501	27/27	0.88	0.21	-0.09	64,77,148,194	0

6.5 Other polymers

There are no such residues in this entry.