Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 – 01:47 PM BST

PDB ID	:	4AIP
Title	:	The FrpB iron transporter from Neisseria meningitidis (F3-3 variant)
Authors	:	Saleem, M.; Prince, S.M.; Derrick, J.P.
Deposited on	:	2012-02-11
Resolution	:	2.40 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 (i) symbol.

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

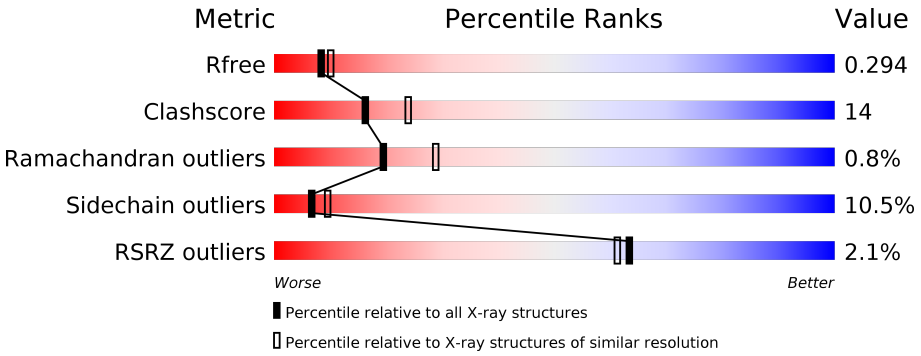
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	742	61% 22% 5% • 11%
1	B	742	3% 61% 23% • • 10%
1	C	742	2% 61% 23% 5% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15985 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 FE-REGULATED PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5178	3234	944	995	5			
1	B	665	Total	C	N	O	S	0	0	0
			5209	3247	956	1002	4			
1	C	665	Total	C	N	O	S	0	0	0
			5212	3253	952	1002	5			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q51162
A	2	HIS	-	expression tag	UNP Q51162
A	3	HIS	-	expression tag	UNP Q51162
A	4	HIS	-	expression tag	UNP Q51162
A	5	HIS	-	expression tag	UNP Q51162
A	6	HIS	-	expression tag	UNP Q51162
A	7	HIS	-	expression tag	UNP Q51162
A	8	SER	-	expression tag	UNP Q51162
A	9	SER	-	expression tag	UNP Q51162
A	10	GLY	-	expression tag	UNP Q51162
A	11	LEU	-	expression tag	UNP Q51162
A	12	VAL	-	expression tag	UNP Q51162
A	13	PRO	-	expression tag	UNP Q51162
A	14	ARG	-	expression tag	UNP Q51162
A	15	GLY	-	expression tag	UNP Q51162
A	16	SER	-	expression tag	UNP Q51162
A	17	GLY	-	expression tag	UNP Q51162
A	18	MET	-	expression tag	UNP Q51162
A	19	LYS	-	expression tag	UNP Q51162
A	20	GLU	-	expression tag	UNP Q51162
A	21	THR	-	expression tag	UNP Q51162
A	22	ALA	-	expression tag	UNP Q51162
A	23	ALA	-	expression tag	UNP Q51162

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	-	expression tag	UNP Q51162
A	25	LYS	-	expression tag	UNP Q51162
A	26	PHE	-	expression tag	UNP Q51162
A	27	GLU	-	expression tag	UNP Q51162
A	28	ARG	-	expression tag	UNP Q51162
A	29	GLN	-	expression tag	UNP Q51162
A	30	HIS	-	expression tag	UNP Q51162
A	31	MET	-	expression tag	UNP Q51162
A	32	ASP	-	expression tag	UNP Q51162
A	33	SER	-	expression tag	UNP Q51162
A	34	PRO	-	expression tag	UNP Q51162
A	35	ASP	-	expression tag	UNP Q51162
A	36	LEU	-	expression tag	UNP Q51162
A	37	GLY	-	expression tag	UNP Q51162
A	38	THR	-	expression tag	UNP Q51162
A	39	ASP	-	expression tag	UNP Q51162
A	40	ASP	-	expression tag	UNP Q51162
A	41	ASP	-	expression tag	UNP Q51162
A	42	ASP	-	expression tag	UNP Q51162
A	43	LYS	-	expression tag	UNP Q51162
A	44	MET	-	expression tag	UNP Q51162
A	197	ASN	GLU	conflict	UNP Q51162
A	446	ILE	VAL	conflict	UNP Q51162
B	1	MET	-	expression tag	UNP Q51162
B	2	HIS	-	expression tag	UNP Q51162
B	3	HIS	-	expression tag	UNP Q51162
B	4	HIS	-	expression tag	UNP Q51162
B	5	HIS	-	expression tag	UNP Q51162
B	6	HIS	-	expression tag	UNP Q51162
B	7	HIS	-	expression tag	UNP Q51162
B	8	SER	-	expression tag	UNP Q51162
B	9	SER	-	expression tag	UNP Q51162
B	10	GLY	-	expression tag	UNP Q51162
B	11	LEU	-	expression tag	UNP Q51162
B	12	VAL	-	expression tag	UNP Q51162
B	13	PRO	-	expression tag	UNP Q51162
B	14	ARG	-	expression tag	UNP Q51162
B	15	GLY	-	expression tag	UNP Q51162
B	16	SER	-	expression tag	UNP Q51162
B	17	GLY	-	expression tag	UNP Q51162
B	18	MET	-	expression tag	UNP Q51162
B	19	LYS	-	expression tag	UNP Q51162

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	GLU	-	expression tag	UNP Q51162
B	21	THR	-	expression tag	UNP Q51162
B	22	ALA	-	expression tag	UNP Q51162
B	23	ALA	-	expression tag	UNP Q51162
B	24	ALA	-	expression tag	UNP Q51162
B	25	LYS	-	expression tag	UNP Q51162
B	26	PHE	-	expression tag	UNP Q51162
B	27	GLU	-	expression tag	UNP Q51162
B	28	ARG	-	expression tag	UNP Q51162
B	29	GLN	-	expression tag	UNP Q51162
B	30	HIS	-	expression tag	UNP Q51162
B	31	MET	-	expression tag	UNP Q51162
B	32	ASP	-	expression tag	UNP Q51162
B	33	SER	-	expression tag	UNP Q51162
B	34	PRO	-	expression tag	UNP Q51162
B	35	ASP	-	expression tag	UNP Q51162
B	36	LEU	-	expression tag	UNP Q51162
B	37	GLY	-	expression tag	UNP Q51162
B	38	THR	-	expression tag	UNP Q51162
B	39	ASP	-	expression tag	UNP Q51162
B	40	ASP	-	expression tag	UNP Q51162
B	41	ASP	-	expression tag	UNP Q51162
B	42	ASP	-	expression tag	UNP Q51162
B	43	LYS	-	expression tag	UNP Q51162
B	44	MET	-	expression tag	UNP Q51162
B	197	ASN	GLU	conflict	UNP Q51162
B	446	ILE	VAL	conflict	UNP Q51162
C	1	MET	-	expression tag	UNP Q51162
C	2	HIS	-	expression tag	UNP Q51162
C	3	HIS	-	expression tag	UNP Q51162
C	4	HIS	-	expression tag	UNP Q51162
C	5	HIS	-	expression tag	UNP Q51162
C	6	HIS	-	expression tag	UNP Q51162
C	7	HIS	-	expression tag	UNP Q51162
C	8	SER	-	expression tag	UNP Q51162
C	9	SER	-	expression tag	UNP Q51162
C	10	GLY	-	expression tag	UNP Q51162
C	11	LEU	-	expression tag	UNP Q51162
C	12	VAL	-	expression tag	UNP Q51162
C	13	PRO	-	expression tag	UNP Q51162
C	14	ARG	-	expression tag	UNP Q51162
C	15	GLY	-	expression tag	UNP Q51162

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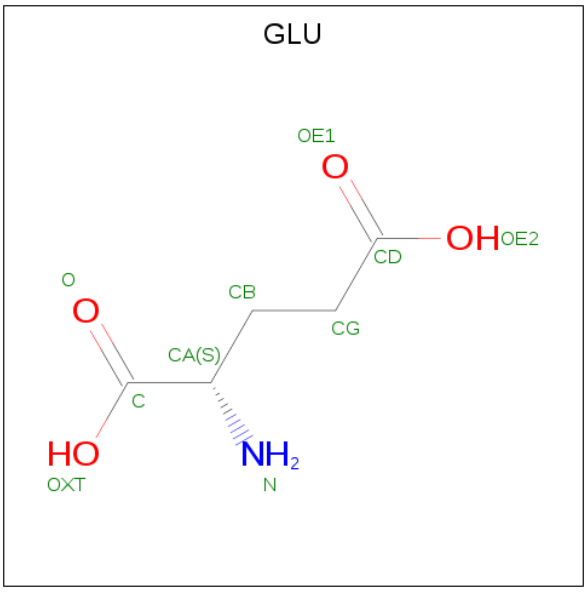
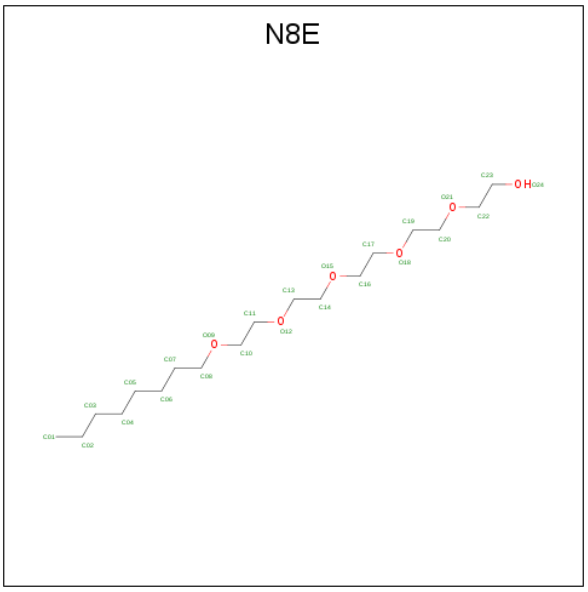
Chain	Residue	Modelled	Actual	Comment	Reference
C	16	SER	-	expression tag	UNP Q51162
C	17	GLY	-	expression tag	UNP Q51162
C	18	MET	-	expression tag	UNP Q51162
C	19	LYS	-	expression tag	UNP Q51162
C	20	GLU	-	expression tag	UNP Q51162
C	21	THR	-	expression tag	UNP Q51162
C	22	ALA	-	expression tag	UNP Q51162
C	23	ALA	-	expression tag	UNP Q51162
C	24	ALA	-	expression tag	UNP Q51162
C	25	LYS	-	expression tag	UNP Q51162
C	26	PHE	-	expression tag	UNP Q51162
C	27	GLU	-	expression tag	UNP Q51162
C	28	ARG	-	expression tag	UNP Q51162
C	29	GLN	-	expression tag	UNP Q51162
C	30	HIS	-	expression tag	UNP Q51162
C	31	MET	-	expression tag	UNP Q51162
C	32	ASP	-	expression tag	UNP Q51162
C	33	SER	-	expression tag	UNP Q51162
C	34	PRO	-	expression tag	UNP Q51162
C	35	ASP	-	expression tag	UNP Q51162
C	36	LEU	-	expression tag	UNP Q51162
C	37	GLY	-	expression tag	UNP Q51162
C	38	THR	-	expression tag	UNP Q51162
C	39	ASP	-	expression tag	UNP Q51162
C	40	ASP	-	expression tag	UNP Q51162
C	41	ASP	-	expression tag	UNP Q51162
C	42	ASP	-	expression tag	UNP Q51162
C	43	LYS	-	expression tag	UNP Q51162
C	44	MET	-	expression tag	UNP Q51162
C	197	ASN	GLU	conflict	UNP Q51162
C	446	ILE	VAL	conflict	UNP Q51162

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		
3	B	1	Total	C	O	0	0
			24	18	6		

- Molecule 4 is water.

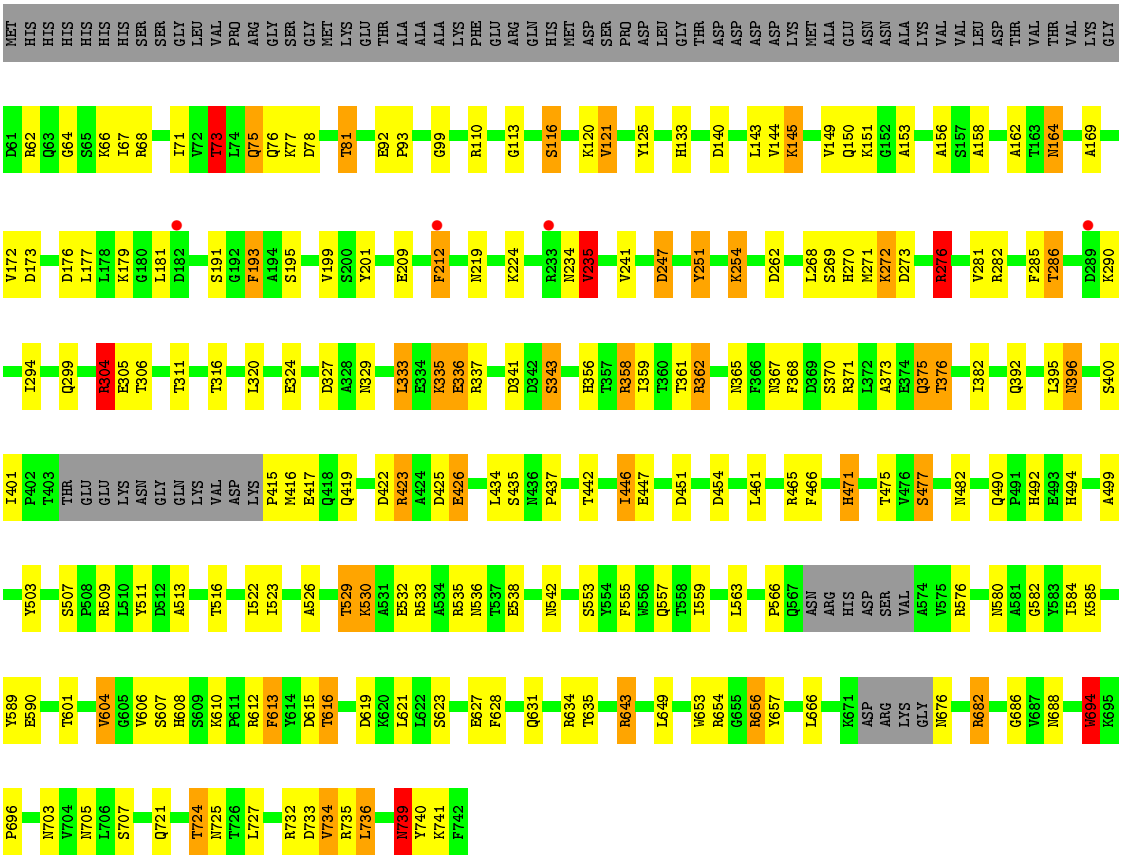
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	133	Total O 133 133	0	0
4	B	80	Total O 80 80	0	0
4	C	115	Total O 115 115	0	0

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.

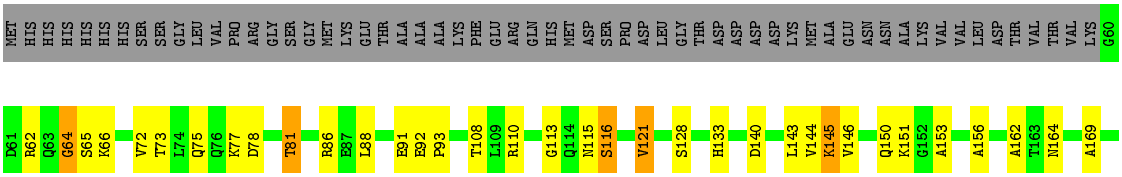
- Molecule 1: FE-REGULATED PROTEIN B

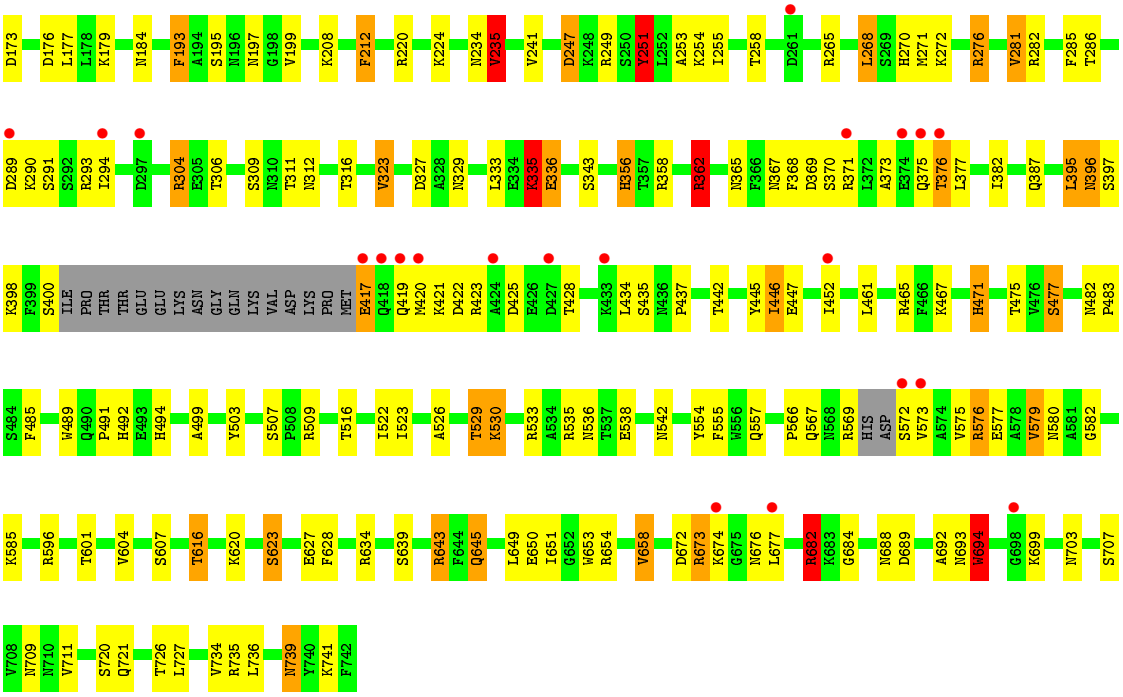
Chain A:



- Molecule 1: FE-REGULATED PROTEIN B

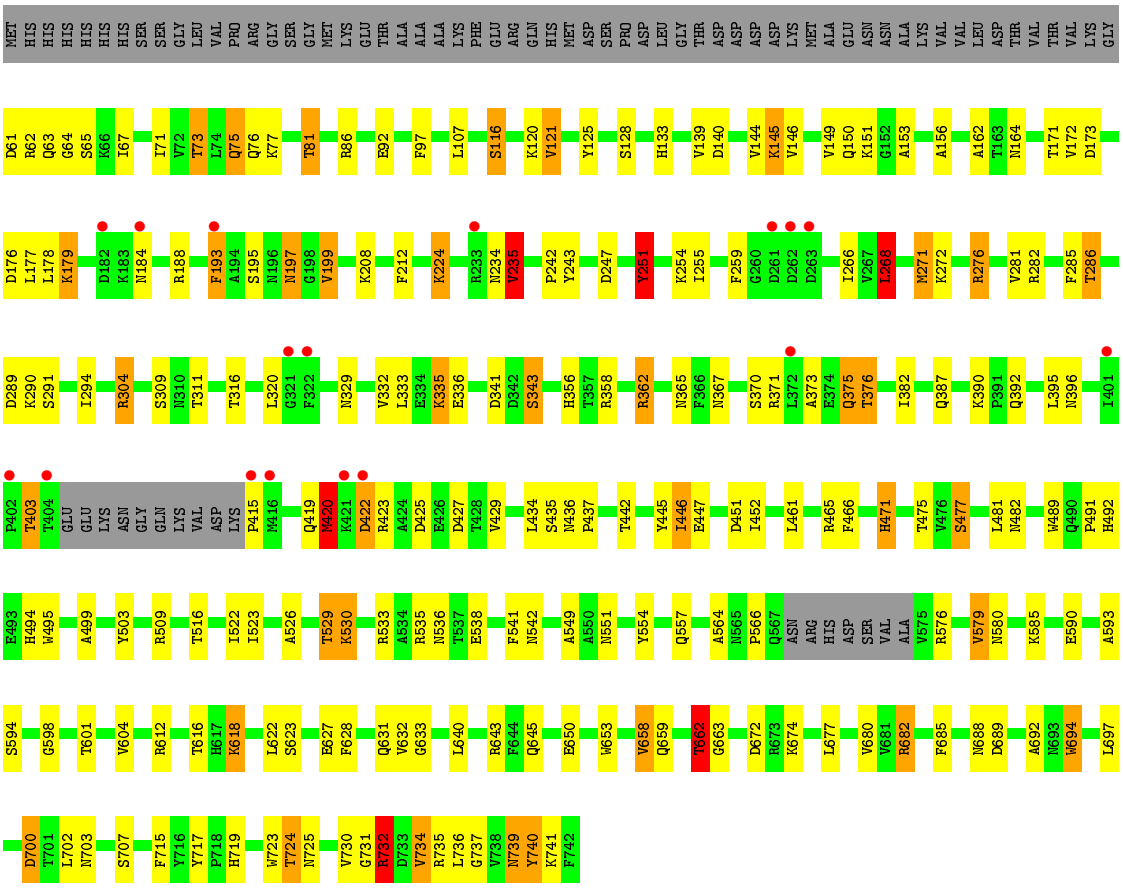
Chain B:





• Molecule 1: FE-REGULATED PROTEIN B

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.32Å 104.62Å 269.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.55 – 2.40 48.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.4 (134.55-2.40) 90.5 (48.76-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.296 0.242 , 0.294	Depositor DCC
R_{free} test set	4316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15985	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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, 0.333 respectively for untwinned datasets, and 0.375, 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: N8E

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	1.24	28/5286 (0.5%)	1.16	36/7135 (0.5%)
1	B	1.17	27/5316 (0.5%)	1.08	27/7173 (0.4%)
1	C	1.23	27/5321 (0.5%)	1.18	43/7182 (0.6%)
All	All	1.21	82/15923 (0.5%)	1.14	106/21490 (0.5%)

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
1	C	0	1
All	All	0	3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	PHE	CB-CG	-16.20	1.23	1.51
1	A	212	PHE	CG-CD1	-15.03	1.16	1.38
1	A	212	PHE	CB-CG	-14.36	1.26	1.51
1	A	212	PHE	CE2-CZ	-12.92	1.12	1.37
1	C	193	PHE	CE1-CZ	-12.31	1.14	1.37
1	B	193	PHE	CB-CG	-10.78	1.33	1.51
1	A	193	PHE	CB-CG	-10.23	1.33	1.51
1	B	212	PHE	CB-CG	-10.01	1.34	1.51
1	C	212	PHE	CB-CG	-9.43	1.35	1.51
1	A	251	TYR	CE1-CZ	-9.33	1.26	1.38
1	B	251	TYR	CD1-CE1	-9.26	1.25	1.39
1	C	62	ARG	CZ-NH1	-9.12	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	PHE	CG-CD1	-8.89	1.25	1.38
1	C	251	TYR	CD1-CE1	-8.75	1.26	1.39
1	A	304	ARG	CZ-NH1	-8.65	1.21	1.33
1	A	358	ARG	CZ-NH2	-8.62	1.21	1.33
1	A	251	TYR	CD2-CE2	-8.58	1.26	1.39
1	B	251	TYR	CB-CG	-8.44	1.39	1.51
1	A	251	TYR	CD1-CE1	-8.16	1.27	1.39
1	A	212	PHE	CD1-CE1	-7.85	1.23	1.39
1	A	212	PHE	CG-CD2	-7.82	1.27	1.38
1	A	193	PHE	CD1-CE1	-7.82	1.23	1.39
1	A	193	PHE	CD2-CE2	-7.81	1.23	1.39
1	C	193	PHE	CG-CD2	-7.73	1.27	1.38
1	B	212	PHE	CG-CD2	-7.38	1.27	1.38
1	B	212	PHE	CD2-CE2	-7.26	1.24	1.39
1	A	73	THR	CB-CG2	-7.24	1.28	1.52
1	C	212	PHE	CG-CD1	-7.13	1.28	1.38
1	C	251	TYR	CB-CG	-7.11	1.41	1.51
1	C	193	PHE	CE2-CZ	-7.09	1.23	1.37
1	C	212	PHE	CG-CD2	-7.06	1.28	1.38
1	B	212	PHE	CD1-CE1	-7.02	1.25	1.39
1	B	251	TYR	CG-CD1	-6.87	1.30	1.39
1	C	336	GLU	CB-CG	-6.85	1.39	1.52
1	B	362	ARG	CZ-NH1	-6.79	1.24	1.33
1	B	212	PHE	CE2-CZ	-6.76	1.24	1.37
1	A	193	PHE	CG-CD1	-6.75	1.28	1.38
1	A	336	GLU	CB-CG	-6.67	1.39	1.52
1	A	269	SER	CB-OG	-6.60	1.33	1.42
1	A	254	LYS	CB-CG	-6.55	1.34	1.52
1	B	73	THR	CB-CG2	-6.37	1.31	1.52
1	B	212	PHE	CG-CD1	-6.37	1.29	1.38
1	A	254	LYS	CE-NZ	-6.29	1.33	1.49
1	A	251	TYR	CB-CG	-6.28	1.42	1.51
1	B	336	GLU	CB-CG	-6.28	1.40	1.52
1	B	193	PHE	CD1-CE1	-6.27	1.26	1.39
1	C	212	PHE	CD1-CE1	-6.23	1.26	1.39
1	B	251	TYR	CE2-CZ	-6.17	1.30	1.38
1	B	485	PHE	CE2-CZ	5.95	1.48	1.37
1	A	212	PHE	CE1-CZ	-5.92	1.26	1.37
1	C	251	TYR	CG-CD1	-5.91	1.31	1.39
1	B	251	TYR	CD2-CE2	-5.86	1.30	1.39
1	C	73	THR	CB-CG2	-5.81	1.33	1.52
1	B	62	ARG	CZ-NH1	-5.78	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	ARG	CZ-NH2	-5.77	1.25	1.33
1	C	375	GLN	CG-CD	-5.76	1.37	1.51
1	C	212	PHE	CE2-CZ	-5.76	1.26	1.37
1	C	212	PHE	CD2-CE2	-5.76	1.27	1.39
1	C	251	TYR	CE2-CZ	-5.74	1.31	1.38
1	A	375	GLN	CG-CD	-5.71	1.38	1.51
1	B	193	PHE	CD2-CE2	-5.67	1.27	1.39
1	B	193	PHE	CG-CD1	-5.61	1.30	1.38
1	A	589	TYR	CD2-CE2	5.61	1.47	1.39
1	C	627	GLU	CB-CG	-5.57	1.41	1.52
1	C	356	HIS	CA-CB	-5.54	1.41	1.53
1	B	417	GLU	CG-CD	5.51	1.60	1.51
1	B	358	ARG	CZ-NH2	-5.49	1.25	1.33
1	A	358	ARG	CZ-NH1	-5.47	1.25	1.33
1	B	477	SER	CB-OG	-5.33	1.35	1.42
1	B	375	GLN	CG-CD	-5.31	1.38	1.51
1	C	212	PHE	CE1-CZ	-5.29	1.27	1.37
1	C	358	ARG	CZ-NH2	-5.29	1.26	1.33
1	B	417	GLU	CB-CG	5.27	1.62	1.52
1	C	740	TYR	CE1-CZ	5.23	1.45	1.38
1	A	62	ARG	CZ-NH1	-5.21	1.26	1.33
1	B	212	PHE	CE1-CZ	-5.21	1.27	1.37
1	C	251	TYR	CD2-CE2	-5.20	1.31	1.39
1	A	193	PHE	CG-CD2	-5.18	1.30	1.38
1	A	286	THR	CB-CG2	-5.16	1.35	1.52
1	C	193	PHE	CD1-CE1	-5.06	1.29	1.39
1	B	254	LYS	CE-NZ	-5.06	1.36	1.49
1	A	367	ASN	CB-CG	-5.02	1.39	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH2	20.36	130.48	120.30
1	B	362	ARG	NE-CZ-NH2	16.90	128.75	120.30
1	A	304	ARG	NE-CZ-NH1	-15.77	112.42	120.30
1	A	358	ARG	NE-CZ-NH1	14.11	127.35	120.30
1	C	193	PHE	CB-CG-CD2	12.50	129.55	120.80
1	A	62	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	C	304	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	C	62	ARG	NE-CZ-NH2	10.96	125.78	120.30
1	C	682	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	C	682	ARG	NE-CZ-NH1	10.05	125.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	B	362	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	C	304	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	C	356	HIS	CB-CA-C	-9.21	91.98	110.40
1	A	212	PHE	CB-CA-C	9.17	128.74	110.40
1	A	140	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	A	371	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	B	371	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	C	193	PHE	CG-CD1-CE1	8.73	130.40	120.80
1	C	335	LYS	CD-CE-NZ	8.56	131.39	111.70
1	A	362	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	C	451	ASP	CB-CG-OD1	8.46	125.91	118.30
1	B	304	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	B	304	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	C	362	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	A	733	ASP	CB-CG-OD1	8.01	125.51	118.30
1	B	254	LYS	CD-CE-NZ	8.00	130.10	111.70
1	C	371	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	62	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	C	62	ARG	NH1-CZ-NH2	-7.61	111.03	119.40
1	C	371	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	C	140	ASP	CB-CG-OD1	7.53	125.08	118.30
1	C	193	PHE	CB-CA-C	-7.48	95.44	110.40
1	A	62	ARG	NH1-CZ-NH2	-7.30	111.38	119.40
1	C	358	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	682	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	461	LEU	CB-CG-CD1	-7.03	99.04	111.00
1	C	509	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	140	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	193	PHE	CG-CD2-CE2	-6.82	113.30	120.80
1	A	451	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	682	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	446	ILE	CB-CA-C	-6.57	98.47	111.60
1	A	656	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	446	ILE	CB-CA-C	-6.52	98.56	111.60
1	C	271	MET	CG-SD-CE	6.34	110.35	100.20
1	A	451	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	C	446	ILE	CB-CA-C	-6.24	99.13	111.60
1	A	643	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	356	HIS	N-CA-CB	-6.16	99.52	110.60
1	C	689	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	B	86	ARG	NE-CZ-NH1	6.09	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	643	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	689	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	193	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	A	276	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	700	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	640	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	C	62	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	251	TYR	CE1-CZ-OH	-5.76	104.54	120.10
1	B	694	TRP	CA-CB-CG	5.74	124.60	113.70
1	B	78	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	739	ASN	CB-CA-C	-5.71	98.97	110.40
1	A	724	THR	C-N-CA	-5.71	107.42	121.70
1	C	73	THR	OG1-CB-CG2	-5.66	96.99	110.00
1	C	193	PHE	CZ-CE2-CD2	5.66	126.89	120.10
1	B	62	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	B	247	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	335	LYS	CD-CE-NZ	5.59	124.56	111.70
1	C	662	THR	C-N-CA	-5.57	110.61	122.30
1	A	273	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	375	GLN	CB-CA-C	-5.50	99.39	110.40
1	C	320	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	212	PHE	CD1-CE1-CZ	5.45	126.64	120.10
1	B	461	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	371	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	251	TYR	CB-CA-C	-5.41	99.58	110.40
1	B	682	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	694	TRP	CA-CB-CG	5.39	123.94	113.70
1	C	663	GLY	N-CA-C	5.38	126.54	113.10
1	B	375	GLN	CB-CA-C	-5.37	99.66	110.40
1	C	732	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	262	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	268	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	281	VAL	N-CA-C	-5.33	96.61	111.00
1	C	197	ASN	N-CA-C	-5.33	96.62	111.00
1	C	140	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	656	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	451	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	78	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	371	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	694	TRP	CA-CB-CG	5.22	123.62	113.70
1	B	467	LYS	CD-CE-NZ	-5.21	99.73	111.70
1	A	396	ASN	N-CA-CB	-5.20	101.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	61	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	335	LYS	CD-CE-NZ	5.14	123.52	111.70
1	C	481	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	739	ASN	N-CA-CB	5.10	119.78	110.60
1	C	579	VAL	CB-CA-C	-5.09	101.73	111.40
1	B	576	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	732	ARG	N-CA-CB	-5.07	101.47	110.60
1	A	604	VAL	CB-CA-C	-5.06	101.78	111.40
1	B	140	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	86	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	197	ASN	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	LEU	Peptide
1	B	395	LEU	Peptide
1	C	395	LEU	Peptide

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	5178	0	5017	165	0
1	B	5209	0	5045	151	0
1	C	5212	0	5053	158	0
2	A	10	0	5	1	0
3	A	24	0	38	4	0
3	B	24	0	38	14	0
4	A	133	0	0	12	0
4	B	80	0	0	7	0
4	C	115	0	0	10	0
All	All	15985	0	15196	445	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 14.

All (445) 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:209:GLU:OE1	1:C:740:TYR:CE1	1.90	1.24
1:A:285:PHE:CB	1:A:294:ILE:HD11	1.75	1.16
1:A:209:GLU:OE1	1:C:740:TYR:CZ	1.97	1.15
1:C:732:ARG:HH11	1:C:732:ARG:CG	1.62	1.08
1:B:285:PHE:CB	1:B:294:ILE:HD11	1.83	1.07
1:B:285:PHE:HB3	1:B:294:ILE:CD1	1.85	1.06
1:C:367:ASN:OD1	1:C:445:TYR:OH	1.74	1.04
1:C:285:PHE:CB	1:C:294:ILE:HD11	1.88	1.03
1:C:285:PHE:HB3	1:C:294:ILE:CD1	1.89	1.03
1:C:242:PRO:O	1:C:286:THR:HG22	1.62	1.00
1:C:732:ARG:HH11	1:C:732:ARG:HG2	1.28	0.98
1:A:285:PHE:HB3	1:A:294:ILE:HD11	0.99	0.97
1:A:193:PHE:CE1	1:B:311:THR:HG21	1.99	0.97
1:A:285:PHE:HB3	1:A:294:ILE:CD1	1.94	0.96
1:C:304:ARG:HD2	4:C:2079:HOH:O	1.64	0.95
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.32	0.94
1:B:362:ARG:HH11	1:B:362:ARG:CG	1.77	0.94
1:B:736:LEU:CD2	1:C:268:LEU:HD11	1.99	0.93
1:C:732:ARG:NH1	1:C:732:ARG:CG	2.25	0.92
1:C:177:LEU:O	1:C:741:LYS:HE3	1.70	0.92
1:C:612:ARG:HH12	1:C:631:GLN:NE2	1.68	0.92
1:B:255:ILE:HB	3:B:1743:N8E:H141	1.53	0.91
1:B:645:GLN:OE1	1:B:645:GLN:HA	1.70	0.90
1:B:81:THR:HG23	1:B:735:ARG:HD3	1.53	0.89
1:C:281:VAL:O	1:C:282:ARG:HB2	1.74	0.88
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.37	0.87
1:C:285:PHE:HB3	1:C:294:ILE:HD11	0.94	0.87
1:C:471:HIS:HE1	1:C:523:ILE:H	1.23	0.86
1:B:281:VAL:O	1:B:282:ARG:HB2	1.76	0.85
1:A:471:HIS:HE1	1:A:523:ILE:H	1.24	0.85
1:B:471:HIS:HE1	1:B:523:ILE:H	1.22	0.84
1:B:396:ASN:HD21	1:B:434:LEU:HG	1.40	0.84
1:C:64:GLY:H	1:C:542:ASN:HD21	1.25	0.83
1:C:601:THR:HG22	4:C:2102:HOH:O	1.77	0.83
1:C:653:TRP:HE1	1:C:688:ASN:HD22	1.21	0.83
1:C:612:ARG:HH12	1:C:631:GLN:HE21	1.27	0.82
1:C:732:ARG:NH1	1:C:732:ARG:HG3	1.91	0.82
1:B:285:PHE:HB3	1:B:294:ILE:HD11	0.90	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:NH1	1:A:426:GLU:OE2	2.14	0.81
1:B:703:ASN:HD22	1:B:739:ASN:HD21	1.29	0.81
1:A:268:LEU:HD22	1:C:193:PHE:CE2	2.15	0.80
1:C:242:PRO:O	1:C:286:THR:CG2	2.30	0.80
1:B:736:LEU:HD23	1:C:268:LEU:HD11	1.64	0.79
1:B:367:ASN:OD1	1:B:445:TYR:OH	1.99	0.79
1:A:281:VAL:O	1:A:282:ARG:HB2	1.82	0.79
1:A:81:THR:HG23	1:A:735:ARG:HD3	1.62	0.79
1:B:672:ASP:O	1:B:674:LYS:N	2.15	0.79
1:B:212:PHE:HB3	3:B:1743:N8E:H231	1.67	0.76
1:A:530:LYS:H	1:A:580:ASN:HD21	1.32	0.76
1:A:64:GLY:H	1:A:542:ASN:HD21	1.31	0.75
1:C:471:HIS:CE1	1:C:523:ILE:H	2.05	0.75
1:A:423:ARG:HG3	1:A:423:ARG:NH1	2.01	0.75
1:A:201:TYR:HE1	3:B:1743:N8E:H013	1.52	0.74
1:A:703:ASN:HD22	1:A:739:ASN:ND2	1.85	0.74
1:C:419:GLN:O	1:C:422:ASP:HB2	1.87	0.74
1:A:471:HIS:CE1	1:A:523:ILE:H	2.05	0.73
1:B:251:TYR:HE1	1:B:272:LYS:HD2	1.53	0.72
1:B:653:TRP:HE1	1:B:688:ASN:HD22	1.37	0.72
1:B:582:GLY:HA2	1:B:616:THR:HB	1.72	0.71
1:A:193:PHE:CD1	1:B:311:THR:HG21	2.26	0.71
1:A:268:LEU:HD13	1:C:193:PHE:CD1	2.25	0.71
1:A:362:ARG:HB3	3:A:1743:N8E:H042	1.73	0.71
1:C:434:LEU:HD21	1:C:522:ILE:HD11	1.72	0.71
1:A:434:LEU:HD21	1:A:522:ILE:HD11	1.73	0.70
1:B:177:LEU:O	1:B:741:LYS:HE3	1.90	0.70
1:B:471:HIS:CE1	1:B:523:ILE:H	2.09	0.70
1:A:304:ARG:HB2	1:A:304:ARG:HH11	1.56	0.70
1:B:396:ASN:HD21	1:B:434:LEU:CG	2.04	0.70
1:A:92:GLU:HG3	4:A:2030:HOH:O	1.90	0.69
1:B:672:ASP:C	1:B:674:LYS:H	1.95	0.69
1:A:566:PRO:HB2	1:A:576:ARG:HB3	1.75	0.69
1:B:156:ALA:HB3	1:B:447:GLU:HG3	1.75	0.69
1:B:396:ASN:ND2	1:B:434:LEU:HD12	2.08	0.68
1:A:423:ARG:CG	1:A:423:ARG:HH11	2.07	0.68
1:B:596:ARG:HG2	1:B:601:THR:HG22	1.74	0.68
1:C:403:THR:O	1:C:415:PRO:O	2.11	0.68
1:A:116:SER:HB2	1:A:164:ASN:HB2	1.76	0.68
1:B:65:SER:O	1:B:151:LYS:HE3	1.94	0.67
1:A:285:PHE:CG	1:A:294:ILE:HD11	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ALA:CB	3:B:1743:N8E:H062	2.25	0.67
1:A:336:GLU:HG3	1:A:358:ARG:HG2	1.76	0.66
1:B:270:HIS:HD2	3:B:1743:N8E:H052	1.61	0.66
1:A:209:GLU:OE1	1:C:740:TYR:OH	2.13	0.66
1:B:81:THR:CG2	1:B:735:ARG:HD3	2.25	0.66
1:C:234:ASN:O	1:C:235:VAL:HB	1.94	0.66
1:C:156:ALA:HB3	1:C:447:GLU:HG3	1.78	0.66
1:B:649:LEU:HD13	1:B:694:TRP:HB3	1.78	0.66
1:A:81:THR:HG22	4:A:2015:HOH:O	1.94	0.65
1:B:116:SER:HB2	1:B:164:ASN:HB2	1.79	0.65
1:B:336:GLU:OE1	1:B:356:HIS:CE1	2.49	0.65
1:B:396:ASN:ND2	1:B:434:LEU:CD1	2.60	0.64
1:B:573:VAL:HG22	1:B:576:ARG:HE	1.62	0.64
1:C:434:LEU:HD21	1:C:522:ILE:CD1	2.26	0.64
1:A:219:ASN:HB3	4:A:2068:HOH:O	1.97	0.64
1:B:193:PHE:CD1	1:C:311:THR:HG21	2.33	0.64
1:A:434:LEU:HD21	1:A:522:ILE:CD1	2.28	0.64
1:B:77:LYS:HE3	4:B:2033:HOH:O	1.98	0.64
1:C:73:THR:HG23	1:C:76:GLN:H	1.63	0.64
1:C:164:ASN:ND2	1:C:557:GLN:HE21	1.95	0.64
1:B:682:ARG:NH2	1:B:721:GLN:O	2.31	0.64
1:B:64:GLY:H	1:B:542:ASN:HD21	1.46	0.63
1:C:612:ARG:NH1	1:C:631:GLN:HE21	1.96	0.63
1:C:234:ASN:O	1:C:235:VAL:CB	2.47	0.63
1:C:682:ARG:HD2	4:C:2107:HOH:O	1.97	0.63
1:A:164:ASN:ND2	1:A:557:GLN:HE21	1.97	0.63
1:A:191:SER:HB2	3:B:1743:N8E:H082	1.81	0.63
1:C:153:ALA:HA	1:C:162:ALA:O	1.99	0.63
1:A:145:LYS:HD2	1:A:176:ASP:OD2	1.99	0.63
1:A:612:ARG:HH12	1:A:631:GLN:HE21	1.47	0.63
1:C:672:ASP:O	1:C:674:LYS:N	2.33	0.62
1:B:164:ASN:ND2	1:B:557:GLN:HE21	1.97	0.62
1:A:401:ILE:O	1:A:423:ARG:NH2	2.32	0.62
1:A:304:ARG:HE	1:A:337:ARG:HH21	1.46	0.62
1:B:304:ARG:HD2	4:B:2052:HOH:O	1.99	0.62
1:B:434:LEU:HD21	1:B:522:ILE:CD1	2.30	0.62
1:B:736:LEU:HD21	1:C:268:LEU:HD11	1.82	0.62
1:A:268:LEU:HD13	1:C:193:PHE:CE1	2.34	0.61
1:C:251:TYR:HE1	1:C:272:LYS:HD2	1.65	0.61
1:B:566:PRO:HG2	1:B:576:ARG:HD2	1.82	0.61
1:A:172:VAL:O	1:A:254:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:HIS:CD2	1:B:494:HIS:H	2.19	0.61
1:A:329:ASN:HD22	1:A:365:ASN:HD22	1.49	0.61
1:B:434:LEU:HD21	1:B:522:ILE:HD11	1.83	0.60
1:A:66:LYS:HD2	1:A:538:GLU:CD	2.22	0.60
1:B:92:GLU:HG3	4:B:2011:HOH:O	2.00	0.60
1:B:536:ASN:HB2	1:B:557:GLN:OE1	2.01	0.60
1:B:482:ASN:ND2	1:B:533:ARG:HE	2.00	0.60
1:C:73:THR:CG2	1:C:76:GLN:HG3	2.32	0.60
1:A:247:ASP:HB3	1:A:276:ARG:HG2	1.83	0.60
1:A:81:THR:HG21	1:A:707:SER:OG	2.01	0.60
1:C:121:VAL:HG21	1:C:271:MET:CE	2.32	0.60
1:C:64:GLY:N	1:C:542:ASN:HD21	1.97	0.59
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.14	0.59
1:B:270:HIS:CD2	3:B:1743:N8E:H052	2.37	0.59
1:A:703:ASN:HD22	1:A:739:ASN:HD21	1.47	0.59
1:A:471:HIS:HD2	1:A:516:THR:O	1.86	0.59
1:B:293:ARG:HD2	1:B:673:ARG:NE	2.18	0.59
1:A:177:LEU:O	1:A:741:LYS:HE3	2.03	0.59
1:A:492:HIS:CD2	1:A:494:HIS:H	2.19	0.59
1:A:482:ASN:ND2	1:A:533:ARG:HE	2.01	0.59
1:C:466:PHE:O	1:C:477:SER:HB3	2.03	0.59
1:C:77:LYS:NZ	1:C:144:VAL:O	2.36	0.59
1:C:662:THR:O	1:C:680:VAL:O	2.20	0.59
1:A:156:ALA:HB3	1:A:447:GLU:HG3	1.84	0.58
1:A:582:GLY:HA2	1:A:616:THR:HB	1.85	0.58
1:A:492:HIS:HD2	1:A:494:HIS:H	1.52	0.58
1:B:419:GLN:O	1:B:422:ASP:N	2.36	0.58
1:A:304:ARG:CG	1:A:304:ARG:HH11	2.16	0.58
1:A:536:ASN:HB2	1:A:557:GLN:OE1	2.04	0.57
1:A:120:LYS:HG2	1:A:125:TYR:CD1	2.40	0.57
1:B:425:ASP:OD2	1:B:572:SER:N	2.37	0.57
1:B:91:GLU:OE2	1:B:639:SER:HB3	2.04	0.57
1:C:702:LEU:HD13	1:C:740:TYR:HB2	1.85	0.57
1:A:304:ARG:HE	1:A:337:ARG:NH2	2.02	0.57
1:B:471:HIS:HD2	1:B:516:THR:O	1.88	0.57
1:A:77:LYS:NZ	1:A:144:VAL:O	2.38	0.57
1:B:193:PHE:CE1	1:C:311:THR:HG21	2.40	0.57
1:A:373:ALA:HB3	1:A:376:THR:HG23	1.86	0.57
1:B:336:GLU:OE1	1:B:356:HIS:HE1	1.85	0.57
1:A:270:HIS:HB2	1:C:199:VAL:HG21	1.87	0.57
1:C:373:ALA:HB3	1:C:376:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:O	1:A:235:VAL:CB	2.53	0.56
1:B:329:ASN:HD22	1:B:365:ASN:HD22	1.54	0.56
1:C:281:VAL:O	1:C:282:ARG:CB	2.45	0.56
1:B:492:HIS:HD2	1:B:494:HIS:H	1.53	0.56
1:C:81:THR:HG23	1:C:735:ARG:HD3	1.87	0.56
1:A:740:TYR:CD2	3:B:1743:N8E:H202	2.40	0.56
1:C:145:LYS:HD2	1:C:176:ASP:OD2	2.06	0.56
1:A:110:ARG:HD3	1:A:555:PHE:CZ	2.41	0.56
1:B:234:ASN:O	1:B:235:VAL:CB	2.53	0.56
1:A:234:ASN:O	1:A:235:VAL:HB	2.05	0.56
1:A:612:ARG:HH12	1:A:631:GLN:NE2	2.03	0.56
1:C:121:VAL:HG21	1:C:271:MET:HE1	1.87	0.56
1:C:492:HIS:CD2	1:C:494:HIS:H	2.23	0.56
1:A:657:TYR:CE1	1:A:686:GLY:HA3	2.40	0.55
1:C:195:SER:HB3	1:C:734:VAL:HG13	1.87	0.55
1:C:503:TYR:CZ	1:C:535:ARG:HG3	2.41	0.55
1:B:503:TYR:CZ	1:B:535:ARG:HG3	2.41	0.55
1:C:471:HIS:HD2	1:C:516:THR:O	1.88	0.55
1:C:164:ASN:HD21	1:C:557:GLN:HE21	1.53	0.55
1:C:251:TYR:HD1	1:C:272:LYS:HB3	1.72	0.55
1:B:567:GLN:CD	1:B:579:VAL:HG11	2.27	0.55
1:C:128:SER:OG	1:C:387:GLN:NE2	2.39	0.55
3:A:1743:N8E:H162	1:C:734:VAL:HG22	1.89	0.55
1:A:654:ARG:HD2	4:A:2122:HOH:O	2.06	0.54
1:C:650:GLU:O	1:C:692:ALA:HA	2.07	0.54
1:B:153:ALA:HB3	1:B:536:ASN:HB3	1.89	0.54
1:B:77:LYS:NZ	1:B:144:VAL:O	2.40	0.54
1:C:566:PRO:HB2	1:C:576:ARG:HB3	1.90	0.54
1:A:209:GLU:OE1	1:C:740:TYR:HE1	1.79	0.54
1:A:362:ARG:HH11	1:A:362:ARG:HG2	1.73	0.54
1:C:362:ARG:HH11	1:C:362:ARG:HG2	1.73	0.54
1:B:654:ARG:HD2	4:B:2077:HOH:O	2.08	0.54
1:A:503:TYR:CZ	1:A:535:ARG:HG3	2.42	0.54
1:B:419:GLN:O	1:B:420:MET:C	2.44	0.54
1:B:241:VAL:CG1	1:B:286:THR:HG21	2.38	0.54
1:A:613:PHE:CD1	1:A:613:PHE:N	2.75	0.53
1:A:736:LEU:HD22	1:B:268:LEU:CD1	2.38	0.53
1:C:329:ASN:HD22	1:C:365:ASN:HD22	1.55	0.53
1:B:538:GLU:HB2	1:B:554:TYR:O	2.08	0.53
1:B:672:ASP:OD1	1:B:676:ASN:HB2	2.08	0.53
1:C:392:GLN:HB3	4:C:2082:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB3	1:A:734:VAL:HG13	1.90	0.53
1:C:672:ASP:OD1	1:C:672:ASP:O	2.27	0.53
1:B:234:ASN:O	1:B:235:VAL:HG12	2.09	0.53
1:C:529:THR:HA	1:C:580:ASN:HD21	1.73	0.53
1:B:293:ARG:HD2	1:B:673:ARG:CZ	2.37	0.53
1:A:268:LEU:HD22	1:C:193:PHE:CZ	2.42	0.53
1:A:153:ALA:HB3	1:A:536:ASN:HB3	1.91	0.53
1:B:253:ALA:HB3	3:B:1743:N8E:H062	1.91	0.53
1:A:201:TYR:CE1	3:B:1743:N8E:H013	2.39	0.53
1:C:184:ASN:ND2	1:C:208:LYS:HE3	2.23	0.53
1:B:234:ASN:O	1:B:235:VAL:HB	2.09	0.53
1:B:530:LYS:H	1:B:580:ASN:HD21	1.58	0.52
1:C:549:ALA:O	1:C:593:ALA:HA	2.09	0.52
1:A:653:TRP:HE1	1:A:688:ASN:HD22	1.55	0.52
1:C:612:ARG:HH22	1:C:631:GLN:HE21	1.57	0.52
1:A:419:GLN:O	1:A:423:ARG:HD2	2.09	0.52
1:A:64:GLY:N	1:A:542:ASN:HD21	2.04	0.52
1:C:633:GLY:HA3	1:C:659:GLN:O	2.10	0.52
1:A:66:LYS:HB2	1:A:538:GLU:OE2	2.09	0.52
1:B:153:ALA:HA	1:B:162:ALA:O	2.10	0.52
1:B:526:ALA:O	1:B:529:THR:CG2	2.58	0.52
1:C:75:GLN:NE2	1:C:700:ASP:OD2	2.43	0.52
1:A:241:VAL:CG1	1:A:286:THR:HG21	2.40	0.51
1:C:65:SER:O	1:C:151:LYS:HE3	2.11	0.51
1:A:153:ALA:HA	1:A:162:ALA:O	2.10	0.51
1:A:304:ARG:HD2	4:A:2082:HOH:O	2.11	0.51
1:C:482:ASN:ND2	1:C:533:ARG:HE	2.09	0.51
1:A:281:VAL:O	1:A:299:GLN:OE1	2.29	0.51
1:A:133:HIS:CG	1:A:282:ARG:HG2	2.46	0.51
1:C:717:TYR:CZ	1:C:725:ASN:HB3	2.46	0.51
1:A:270:HIS:CD2	1:C:199:VAL:HG11	2.46	0.50
1:A:286:THR:O	1:A:294:ILE:HG12	2.11	0.50
1:B:115:ASN:HB2	1:B:627:GLU:HG2	1.93	0.50
1:B:113:GLY:HA3	1:B:627:GLU:O	2.11	0.50
1:A:499:ALA:HA	1:A:538:GLU:O	2.10	0.50
1:B:420:MET:O	1:B:423:ARG:N	2.44	0.50
1:A:606:VAL:HA	1:A:635:THR:O	2.11	0.50
1:A:682:ARG:HD2	4:A:2119:HOH:O	2.11	0.50
1:B:286:THR:HG23	1:B:727:LEU:HD21	1.94	0.50
3:A:1743:N8E:H132	1:C:193:PHE:HB3	1.92	0.50
1:A:359:ILE:HD11	1:A:513:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ALA:HB3	1:B:376:THR:HG23	1.92	0.50
1:A:241:VAL:HG12	1:A:286:THR:HG21	1.94	0.50
1:B:286:THR:HG23	1:B:727:LEU:CD2	2.42	0.50
1:B:220:ARG:HG3	1:B:249:ARG:HG2	1.93	0.50
1:B:93:PRO:HB2	1:B:607:SER:HB3	1.93	0.50
1:C:247:ASP:HB3	1:C:276:ARG:HG2	1.94	0.49
1:C:63:GLN:OE1	1:C:67:ILE:HD12	2.12	0.49
1:C:73:THR:HG22	1:C:76:GLN:CG	2.41	0.49
1:B:437:PRO:HG3	1:B:471:HIS:HB3	1.93	0.49
1:C:71:ILE:HD11	1:C:149:VAL:HG12	1.93	0.49
1:C:422:ASP:O	1:C:425:ASP:N	2.46	0.49
1:C:81:THR:HG21	1:C:707:SER:OG	2.12	0.49
1:B:164:ASN:HD21	1:B:557:GLN:HE21	1.59	0.49
1:C:120:LYS:HG2	1:C:125:TYR:CD1	2.48	0.49
1:C:116:SER:HB2	1:C:164:ASN:HB2	1.94	0.49
1:A:657:TYR:CD1	1:A:686:GLY:HA3	2.46	0.49
1:B:688:ASN:O	1:B:711:VAL:HG23	2.13	0.49
1:B:649:LEU:CD1	1:B:694:TRP:HB3	2.43	0.49
1:C:530:LYS:H	1:C:580:ASN:HD21	1.61	0.49
1:B:108:THR:HG23	1:B:720:SER:HB3	1.95	0.49
1:A:530:LYS:N	1:A:580:ASN:HD21	2.05	0.49
1:B:281:VAL:O	1:B:282:ARG:CB	2.46	0.49
1:B:81:THR:HG21	1:B:707:SER:OG	2.12	0.49
1:A:234:ASN:O	1:A:235:VAL:HG12	2.13	0.49
1:B:184:ASN:ND2	1:B:208:LYS:HE3	2.28	0.48
1:B:526:ALA:O	1:B:529:THR:HG23	2.14	0.48
1:A:268:LEU:HB3	1:C:193:PHE:CZ	2.47	0.48
1:C:658:VAL:HG13	1:C:685:PHE:CE1	2.48	0.48
1:C:77:LYS:HE2	4:C:2006:HOH:O	2.11	0.48
1:A:73:THR:HG22	1:A:76:GLN:H	1.78	0.48
1:B:362:ARG:NH1	1:B:362:ARG:CG	2.54	0.48
1:B:672:ASP:C	1:B:674:LYS:N	2.64	0.48
1:C:341:ASP:OD1	1:C:343:SER:OG	2.31	0.48
1:C:92:GLU:HG3	4:C:2022:HOH:O	2.12	0.48
1:A:71:ILE:HD11	1:A:149:VAL:HG12	1.95	0.48
3:A:1743:N8E:H132	1:C:193:PHE:CD2	2.49	0.48
4:A:2074:HOH:O	3:B:1743:N8E:H011	2.14	0.48
1:B:736:LEU:HD21	1:C:268:LEU:CD1	2.42	0.48
1:C:197:ASN:HB3	1:C:224:LYS:HB2	1.95	0.48
1:A:195:SER:CB	1:A:734:VAL:HG13	2.44	0.48
1:C:437:PRO:HG3	1:C:471:HIS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ASN:O	1:A:736:LEU:HA	2.14	0.48
1:B:703:ASN:HD22	1:B:739:ASN:ND2	2.05	0.48
1:B:145:LYS:HD2	1:B:176:ASP:OD2	2.13	0.47
1:B:66:LYS:HB2	1:B:538:GLU:OE2	2.15	0.47
1:A:608:HIS:HE1	4:A:2116:HOH:O	1.97	0.47
1:A:623:SER:HB3	1:A:628:PHE:CE2	2.50	0.47
1:A:694:TRP:O	1:A:696:PRO:HD3	2.15	0.47
1:A:99:GLY:H	1:A:721:GLN:NE2	2.12	0.47
1:A:99:GLY:H	1:A:721:GLN:HE22	1.62	0.47
1:A:191:SER:HB2	3:B:1743:N8E:H102	1.95	0.47
1:B:133:HIS:CG	1:B:282:ARG:HG2	2.50	0.47
1:A:286:THR:HG23	1:A:727:LEU:CD2	2.44	0.47
1:B:251:TYR:HD1	1:B:272:LYS:HB3	1.80	0.46
1:C:390:LYS:HG2	1:C:436:ASN:ND2	2.30	0.46
1:B:247:ASP:HB3	1:B:276:ARG:HG2	1.97	0.46
1:A:145:LYS:HB3	1:A:172:VAL:HA	1.98	0.46
1:C:425:ASP:O	1:C:429:VAL:HG23	2.15	0.46
1:C:492:HIS:HD2	1:C:494:HIS:HB2	1.81	0.46
1:C:612:ARG:NH1	1:C:631:GLN:NE2	2.49	0.46
1:A:268:LEU:HD22	1:C:193:PHE:CD2	2.49	0.46
1:A:415:PRO:O	1:A:419:GLN:HG3	2.16	0.46
1:C:492:HIS:HD2	1:C:494:HIS:H	1.63	0.46
1:B:736:LEU:CD2	1:C:268:LEU:CD1	2.83	0.46
1:A:110:ARG:HD3	1:A:555:PHE:CE2	2.51	0.46
1:A:613:PHE:HD1	1:A:613:PHE:N	2.15	0.45
1:A:682:ARG:NH2	1:A:721:GLN:O	2.49	0.45
1:B:689:ASP:OD1	1:B:709:ASN:HA	2.16	0.45
1:B:72:VAL:HG11	1:B:88:LEU:HD21	1.97	0.45
1:C:672:ASP:O	1:C:672:ASP:CG	2.53	0.45
1:A:164:ASN:HD21	1:A:557:GLN:HE21	1.63	0.45
1:B:64:GLY:N	1:B:542:ASN:HD21	2.12	0.45
1:C:632:VAL:HG13	1:C:719:HIS:HB2	1.99	0.45
1:B:121:VAL:HA	1:B:169:ALA:O	2.16	0.45
1:C:658:VAL:CG1	1:C:685:PHE:CZ	2.99	0.45
1:B:643:ARG:NH2	1:B:693:ASN:OD1	2.46	0.45
1:A:503:TYR:CE2	1:A:535:ARG:HG3	2.52	0.45
1:B:253:ALA:HB2	3:B:1743:N8E:H062	1.98	0.45
1:C:133:HIS:CG	1:C:282:ARG:HG2	2.52	0.45
1:C:499:ALA:HA	1:C:538:GLU:O	2.17	0.45
1:A:466:PHE:O	1:A:477:SER:HB3	2.17	0.45
1:A:113:GLY:HA3	1:A:627:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:HG3	1:C:243:TYR:OH	2.17	0.45
1:C:536:ASN:HB2	1:C:557:GLN:OE1	2.17	0.45
1:C:703:ASN:HB2	1:C:739:ASN:ND2	2.32	0.45
1:A:616:THR:HG21	4:A:2112:HOH:O	2.17	0.45
1:A:181:LEU:HD21	1:A:741:LYS:HB3	1.98	0.45
1:B:489:TRP:CE2	1:B:491:PRO:HG3	2.52	0.45
1:B:312:ASN:OD1	1:B:329:ASN:OD1	2.34	0.45
1:C:526:ALA:O	1:C:529:THR:CG2	2.65	0.44
1:A:426:GLU:H	1:A:426:GLU:HG2	1.47	0.44
1:B:251:TYR:CD1	3:B:1743:N8E:H031	2.52	0.44
1:B:335:LYS:HD2	4:B:2030:HOH:O	2.18	0.44
1:B:499:ALA:HA	1:B:538:GLU:O	2.16	0.44
1:A:305:GLU:OE1	2:A:1744:GLU:HB2	2.18	0.44
1:A:341:ASP:OD1	1:A:343:SER:OG	2.36	0.44
1:B:658:VAL:O	1:B:684:GLY:HA2	2.18	0.44
1:A:270:HIS:CB	1:C:199:VAL:HG21	2.47	0.44
1:A:416:MET:SD	1:A:419:GLN:NE2	2.91	0.44
1:A:209:GLU:CD	1:C:740:TYR:OH	2.56	0.44
1:C:492:HIS:HB3	1:C:495:TRP:HD1	1.83	0.44
1:A:736:LEU:HD22	1:B:268:LEU:HD12	1.99	0.44
1:C:332:VAL:O	1:C:332:VAL:HG13	2.18	0.44
1:A:533:ARG:HD3	4:A:2106:HOH:O	2.17	0.44
1:A:610:LYS:HA	1:A:631:GLN:HE22	1.83	0.44
1:B:335:LYS:HB2	1:B:335:LYS:HE2	1.36	0.44
1:C:564:ALA:HB3	1:C:622:LEU:HA	2.00	0.44
1:A:507:SER:O	1:A:509:ARG:NH1	2.51	0.43
1:C:658:VAL:HG13	1:C:685:PHE:CZ	2.53	0.43
1:C:623:SER:HB3	1:C:628:PHE:CE2	2.53	0.43
1:B:195:SER:HB3	1:B:734:VAL:HG13	1.98	0.43
1:A:143:LEU:HD13	1:A:271:MET:SD	2.58	0.43
1:C:730:VAL:HG12	1:C:731:GLY:O	2.18	0.43
1:B:145:LYS:HG2	1:B:146:VAL:HG22	1.99	0.43
1:C:489:TRP:CE2	1:C:491:PRO:HG3	2.53	0.43
1:C:730:VAL:HG23	4:C:2017:HOH:O	2.17	0.43
1:A:285:PHE:CG	1:A:294:ILE:CD1	3.01	0.43
1:A:559:ILE:HB	1:A:584:ILE:HB	2.00	0.43
1:A:703:ASN:HB2	1:A:739:ASN:ND2	2.33	0.43
1:A:437:PRO:HG3	1:A:471:HIS:HB3	2.01	0.43
1:B:110:ARG:HD3	1:B:555:PHE:CZ	2.54	0.43
1:C:151:LYS:NZ	1:C:590:GLU:OE1	2.47	0.43
1:C:549:ALA:HB3	1:C:594:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:HB2	4:B:2023:HOH:O	2.18	0.43
1:A:362:ARG:HG2	1:A:362:ARG:NH1	2.33	0.43
1:A:526:ALA:O	1:A:529:THR:HG23	2.19	0.43
1:A:133:HIS:CD2	1:A:282:ARG:HG2	2.54	0.43
1:A:368:PHE:N	1:A:368:PHE:CD1	2.86	0.43
1:B:323:VAL:HG21	1:B:368:PHE:HB3	2.01	0.43
1:B:726:THR:OG1	1:B:727:LEU:N	2.51	0.43
1:C:503:TYR:CE2	1:C:535:ARG:HG3	2.54	0.43
1:A:333:LEU:HB3	1:A:361:THR:HB	2.00	0.42
1:B:241:VAL:HG13	1:B:286:THR:HG21	1.99	0.42
1:B:289:ASP:OD2	1:B:291:SER:OG	2.29	0.42
1:B:623:SER:HB3	1:B:628:PHE:CE2	2.55	0.42
1:C:541:PHE:O	1:C:551:ASN:HA	2.19	0.42
1:C:736:LEU:HG	1:C:737:GLY:N	2.34	0.42
1:B:286:THR:O	1:B:294:ILE:HG12	2.20	0.42
1:B:369:ASP:HB3	1:B:377:LEU:HD11	2.01	0.42
1:C:259:PHE:HE1	1:C:266:ILE:HD12	1.83	0.42
1:C:251:TYR:CD1	1:C:272:LYS:HB3	2.53	0.42
1:A:193:PHE:CE1	1:B:311:THR:CG2	2.88	0.42
1:B:294:ILE:HD13	1:B:294:ILE:HG21	1.79	0.42
1:C:133:HIS:CD2	1:C:282:ARG:HG2	2.55	0.42
1:C:286:THR:O	1:C:294:ILE:HG12	2.19	0.42
1:C:618:LYS:HE2	1:C:618:LYS:H	1.84	0.42
1:B:234:ASN:O	1:B:235:VAL:CG1	2.67	0.42
1:C:538:GLU:HB2	1:C:554:TYR:O	2.19	0.42
1:C:723:TRP:C	1:C:724:THR:O	2.54	0.42
1:A:281:VAL:O	1:A:282:ARG:CB	2.51	0.42
1:A:422:ASP:O	1:A:425:ASP:HB2	2.20	0.42
1:A:725:ASN:HD22	1:A:725:ASN:HA	1.72	0.42
1:B:128:SER:OG	1:B:387:GLN:NE2	2.53	0.42
1:B:133:HIS:CD2	1:B:282:ARG:HG2	2.55	0.42
1:B:66:LYS:HD2	1:B:538:GLU:CD	2.39	0.42
1:C:71:ILE:HD11	1:C:149:VAL:CG1	2.50	0.42
1:A:71:ILE:HD11	1:A:149:VAL:CG1	2.49	0.42
1:A:375:GLN:CA	1:A:375:GLN:OE1	2.68	0.42
1:B:241:VAL:HG12	1:B:286:THR:HG21	2.01	0.42
1:A:311:THR:HG23	1:C:193:PHE:HE2	1.84	0.42
1:A:454:ASP:HB2	1:A:490:GLN:O	2.19	0.42
1:A:251:TYR:OH	1:A:272:LYS:HE3	2.20	0.42
1:A:67:ILE:HD11	4:A:2004:HOH:O	2.19	0.42
1:A:93:PRO:HB2	1:A:607:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ARG:NH2	1:C:631:GLN:HE21	2.17	0.42
1:B:258:THR:OG1	1:B:265:ARG:NH1	2.50	0.42
1:B:650:GLU:O	1:B:692:ALA:HA	2.20	0.42
1:C:289:ASP:OD2	1:C:291:SER:OG	2.30	0.42
1:C:715:PHE:HA	4:C:2071:HOH:O	2.19	0.41
1:B:396:ASN:HD21	1:B:434:LEU:CD1	2.24	0.41
1:C:139:VAL:HG23	4:C:2076:HOH:O	2.18	0.41
1:A:526:ALA:O	1:A:529:THR:CG2	2.68	0.41
1:B:143:LEU:HD13	1:B:271:MET:SD	2.60	0.41
1:B:507:SER:O	1:B:509:ARG:NH1	2.54	0.41
1:A:532:GLU:HG3	1:A:563:LEU:HD12	2.03	0.41
1:B:282:ARG:HA	4:B:2028:HOH:O	2.19	0.41
1:C:172:VAL:O	1:C:254:LYS:HE2	2.19	0.41
1:B:251:TYR:CD1	1:B:272:LYS:HB3	2.55	0.41
1:A:151:LYS:NZ	1:A:590:GLU:OE1	2.52	0.41
1:A:73:THR:HG22	1:A:75:GLN:N	2.35	0.41
1:B:569:ARG:HD2	1:B:577:GLU:OE2	2.21	0.41
1:B:703:ASN:HB2	1:B:739:ASN:ND2	2.36	0.41
1:C:178:LEU:O	1:C:179:LYS:C	2.59	0.41
1:A:121:VAL:HA	1:A:169:ALA:O	2.21	0.41
1:A:649:LEU:CD1	1:A:694:TRP:HB3	2.50	0.41
1:A:270:HIS:CG	1:C:199:VAL:HG11	2.56	0.41
1:A:613:PHE:HB2	1:A:666:LEU:HD23	2.02	0.41
1:C:171:THR:OG1	1:C:254:LYS:NZ	2.51	0.41
1:A:311:THR:CG2	1:C:193:PHE:HE2	2.34	0.41
1:C:294:ILE:HG21	1:C:294:ILE:HD13	1.78	0.41
1:C:420:MET:O	1:C:423:ARG:HB2	2.20	0.41
1:A:81:THR:CG2	1:A:735:ARG:HD3	2.44	0.41
1:B:567:GLN:HB3	1:B:579:VAL:HG21	2.03	0.41
1:C:616:THR:HG21	4:C:2099:HOH:O	2.20	0.41
1:A:158:ALA:HB2	4:A:2062:HOH:O	2.20	0.40
1:B:395:LEU:O	1:B:398:LYS:HB2	2.21	0.40
1:C:188:ARG:HG3	1:C:741:LYS:HG3	2.03	0.40
1:B:482:ASN:HA	1:B:483:PRO:HD3	1.92	0.40
1:A:529:THR:HA	1:A:580:ASN:ND2	2.36	0.40
1:A:619:ASP:O	1:A:621:LEU:HG	2.22	0.40
1:C:375:GLN:OE1	1:C:375:GLN:N	2.54	0.40
1:C:97:PHE:CE2	1:C:107:LEU:HD12	2.56	0.40

There are no symmetry-related clashes.

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	653/742 (88%)	626 (96%)	23 (4%)	4 (1%)	25	36
1	B	659/742 (89%)	629 (95%)	24 (4%)	6 (1%)	17	25
1	C	659/742 (89%)	623 (94%)	30 (5%)	6 (1%)	17	25
All	All	1971/2226 (88%)	1878 (95%)	77 (4%)	16 (1%)	19	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	VAL
1	A	396	ASN
1	A	724	THR
1	B	235	VAL
1	B	396	ASN
1	C	235	VAL
1	C	396	ASN
1	C	420	MET
1	A	511	TYR
1	B	620	LYS
1	B	673	ARG
1	C	598	GLY
1	C	422	ASP
1	C	724	THR
1	B	421	LYS
1	B	64	GLY

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	542/612 (89%)	482 (89%)	60 (11%)	6 8
1	B	544/612 (89%)	487 (90%)	57 (10%)	7 9
1	C	546/612 (89%)	492 (90%)	54 (10%)	8 11
All	All	1632/1836 (89%)	1461 (90%)	171 (10%)	7 9

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	73	THR
1	A	75	GLN
1	A	81	THR
1	A	116	SER
1	A	121	VAL
1	A	145	LYS
1	A	150	GLN
1	A	164	ASN
1	A	173	ASP
1	A	179	LYS
1	A	199	VAL
1	A	212	PHE
1	A	224	LYS
1	A	235	VAL
1	A	272	LYS
1	A	276	ARG
1	A	290	LYS
1	A	304	ARG
1	A	306	THR
1	A	316	THR
1	A	320	LEU
1	A	324	GLU
1	A	327	ASP
1	A	333	LEU
1	A	335	LYS
1	A	343	SER
1	A	356	HIS
1	A	370	SER
1	A	376	THR
1	A	382	ILE
1	A	400	SER

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Mol	Chain	Res	Type
1	A	417	GLU
1	A	423	ARG
1	A	426	GLU
1	A	435	SER
1	A	442	THR
1	A	446	ILE
1	A	465	ARG
1	A	471	HIS
1	A	475	THR
1	A	477	SER
1	A	529	THR
1	A	530	LYS
1	A	553	SER
1	A	585	LYS
1	A	601	THR
1	A	604	VAL
1	A	613	PHE
1	A	615	ASP
1	A	616	THR
1	A	634	ARG
1	A	643	ARG
1	A	656	ARG
1	A	676	ASN
1	A	694	TRP
1	A	732	ARG
1	A	734	VAL
1	A	736	LEU
1	A	739	ASN
1	B	75	GLN
1	B	81	THR
1	B	116	SER
1	B	121	VAL
1	B	145	LYS
1	B	150	GLN
1	B	173	ASP
1	B	179	LYS
1	B	199	VAL
1	B	224	LYS
1	B	235	VAL
1	B	251	TYR
1	B	268	LEU
1	B	276	ARG

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Mol	Chain	Res	Type
1	B	290	LYS
1	B	306	THR
1	B	309	SER
1	B	316	THR
1	B	323	VAL
1	B	327	ASP
1	B	333	LEU
1	B	335	LYS
1	B	343	SER
1	B	362	ARG
1	B	370	SER
1	B	376	THR
1	B	382	ILE
1	B	397	SER
1	B	400	SER
1	B	417	GLU
1	B	428	THR
1	B	435	SER
1	B	442	THR
1	B	446	ILE
1	B	452	ILE
1	B	465	ARG
1	B	471	HIS
1	B	475	THR
1	B	477	SER
1	B	529	THR
1	B	530	LYS
1	B	575	VAL
1	B	579	VAL
1	B	585	LYS
1	B	604	VAL
1	B	616	THR
1	B	623	SER
1	B	634	ARG
1	B	643	ARG
1	B	645	GLN
1	B	651	ILE
1	B	658	VAL
1	B	677	LEU
1	B	682	ARG
1	B	694	TRP
1	B	699	LYS

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Mol	Chain	Res	Type
1	B	739	ASN
1	C	75	GLN
1	C	81	THR
1	C	116	SER
1	C	121	VAL
1	C	145	LYS
1	C	146	VAL
1	C	150	GLN
1	C	173	ASP
1	C	179	LYS
1	C	199	VAL
1	C	224	LYS
1	C	235	VAL
1	C	251	TYR
1	C	255	ILE
1	C	268	LEU
1	C	276	ARG
1	C	286	THR
1	C	290	LYS
1	C	309	SER
1	C	316	THR
1	C	333	LEU
1	C	335	LYS
1	C	343	SER
1	C	370	SER
1	C	376	THR
1	C	382	ILE
1	C	403	THR
1	C	420	MET
1	C	427	ASP
1	C	435	SER
1	C	442	THR
1	C	446	ILE
1	C	452	ILE
1	C	461	LEU
1	C	465	ARG
1	C	471	HIS
1	C	475	THR
1	C	477	SER
1	C	529	THR
1	C	530	LYS
1	C	579	VAL

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Mol	Chain	Res	Type
1	C	585	LYS
1	C	604	VAL
1	C	618	LYS
1	C	643	ARG
1	C	645	GLN
1	C	658	VAL
1	C	662	THR
1	C	677	LEU
1	C	694	TRP
1	C	697	LEU
1	C	732	ARG
1	C	734	VAL
1	C	739	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	184	ASN
1	A	264	HIS
1	A	329	ASN
1	A	387	GLN
1	A	419	GLN
1	A	471	HIS
1	A	482	ASN
1	A	492	HIS
1	A	494	HIS
1	A	542	ASN
1	A	580	ASN
1	A	608	HIS
1	A	631	GLN
1	A	679	ASN
1	A	688	ASN
1	A	721	GLN
1	A	725	ASN
1	A	739	ASN
1	B	150	GLN
1	B	164	ASN
1	B	184	ASN
1	B	264	HIS
1	B	329	ASN
1	B	356	HIS

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Mol	Chain	Res	Type
1	B	387	GLN
1	B	396	ASN
1	B	471	HIS
1	B	482	ASN
1	B	492	HIS
1	B	494	HIS
1	B	542	ASN
1	B	580	ASN
1	B	688	ASN
1	B	739	ASN
1	C	115	ASN
1	C	164	ASN
1	C	184	ASN
1	C	274	GLN
1	C	329	ASN
1	C	387	GLN
1	C	471	HIS
1	C	482	ASN
1	C	492	HIS
1	C	494	HIS
1	C	542	ASN
1	C	580	ASN
1	C	631	GLN
1	C	645	GLN
1	C	688	ASN
1	C	725	ASN
1	C	739	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	N8E	B	1743	-	23,23,23	0.45	0	22,22,22	0.68	0
2	GLU	A	1744	-	2,9,9	0.53	0	2,11,11	1.14	0
3	N8E	A	1743	-	23,23,23	0.90	0	22,22,22	1.01	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
3	N8E	B	1743	-	-	13/21/21/21	-
2	GLU	A	1744	-	-	2/3/9/9	-
3	N8E	A	1743	-	-	11/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1743	N8E	O09-C10-C11-O12
3	B	1743	N8E	O12-C13-C14-O15
3	B	1743	N8E	O18-C19-C20-O21
3	A	1743	N8E	O18-C19-C20-O21
3	A	1743	N8E	C06-C07-C08-O09
3	A	1743	N8E	O15-C16-C17-O18
2	A	1744	GLU	CA-CB-CG-CD
3	A	1743	N8E	C04-C05-C06-C07
3	B	1743	N8E	C02-C03-C04-C05

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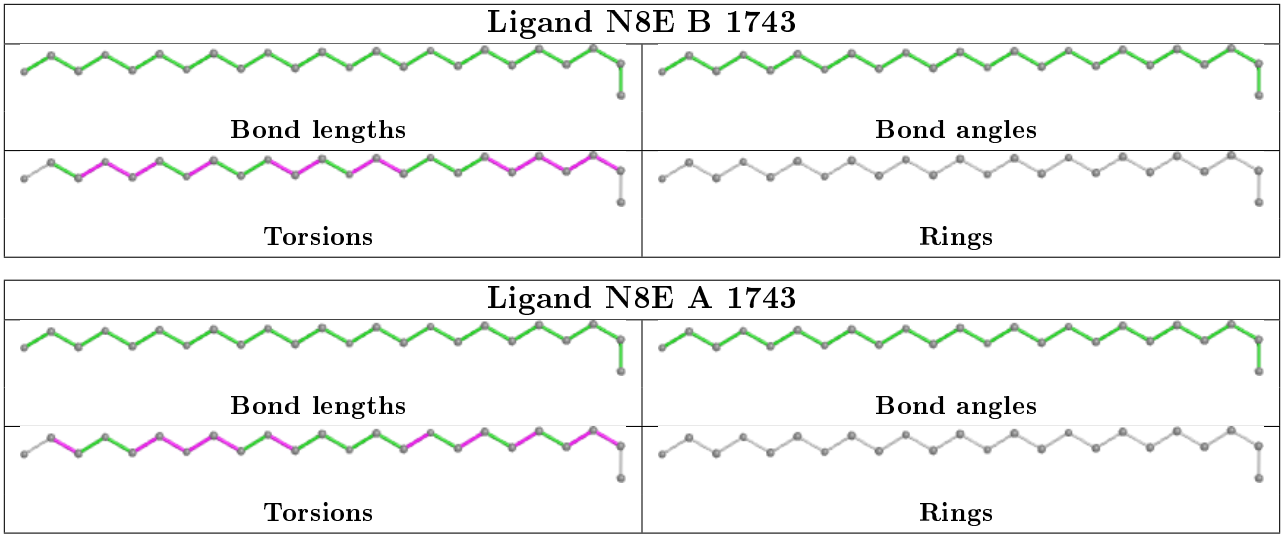
Mol	Chain	Res	Type	Atoms
3	A	1743	N8E	O21-C22-C23-O24
3	A	1743	N8E	C01-C02-C03-C04
3	A	1743	N8E	C02-C03-C04-C05
3	B	1743	N8E	C04-C05-C06-C07
3	B	1743	N8E	C23-C22-O21-C20
3	A	1743	N8E	C20-C19-O18-C17
3	B	1743	N8E	C03-C04-C05-C06
3	B	1743	N8E	C13-C14-O15-C16
3	B	1743	N8E	C16-C17-O18-C19
3	A	1743	N8E	C13-C14-O15-C16
3	B	1743	N8E	C01-C02-C03-C04
3	A	1743	N8E	C11-C10-O09-C08
3	B	1743	N8E	C19-C20-O21-C22
3	B	1743	N8E	C05-C06-C07-C08
3	B	1743	N8E	C10-C11-O12-C13
3	A	1743	N8E	C16-C17-O18-C19
2	A	1744	GLU	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1743	N8E	14	0
2	A	1744	GLU	1	0
3	A	1743	N8E	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	661/742 (89%)	-0.21	4 (0%)	89	88	5, 20, 41, 60	0
1	B	665/742 (89%)	-0.18	21 (3%)	47	46	7, 22, 47, 62	0
1	C	665/742 (89%)	-0.11	17 (2%)	56	54	5, 20, 46, 62	0
All	All	1991/2226 (89%)	-0.17	42 (2%)	63	61	5, 20, 45, 62	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	677	LEU	4.0
1	C	322	PHE	3.9
1	C	261	ASP	3.9
1	C	416	MET	3.6
1	B	420	MET	3.5
1	B	289	ASP	3.3
1	B	294	ILE	3.1
1	C	401	ILE	3.1
1	A	289	ASP	2.9
1	B	427	ASP	2.8
1	C	372	LEU	2.7
1	A	233	ARG	2.7
1	B	419	GLN	2.7
1	C	402	PRO	2.5
1	B	424	ALA	2.5
1	C	263	ASP	2.4
1	C	262	ASP	2.4
1	C	404	THR	2.4
1	C	193	PHE	2.3
1	B	698	GLY	2.3
1	B	374	GLU	2.3
1	B	417	GLU	2.3
1	B	433	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	421	LYS	2.2
1	B	573	VAL	2.2
1	A	212	PHE	2.2
1	B	452	ILE	2.2
1	A	182	ASP	2.2
1	B	572	SER	2.2
1	B	261	ASP	2.2
1	C	321	GLY	2.2
1	B	371	ARG	2.2
1	C	182	ASP	2.1
1	C	415	PRO	2.1
1	B	297	ASP	2.1
1	C	422	ASP	2.1
1	B	418	GLN	2.1
1	B	376	THR	2.1
1	B	674	LYS	2.1
1	C	233	ARG	2.0
1	B	375	GLN	2.0
1	C	184	ASN	2.0

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 monosaccharides in this entry.

6.4 Ligands

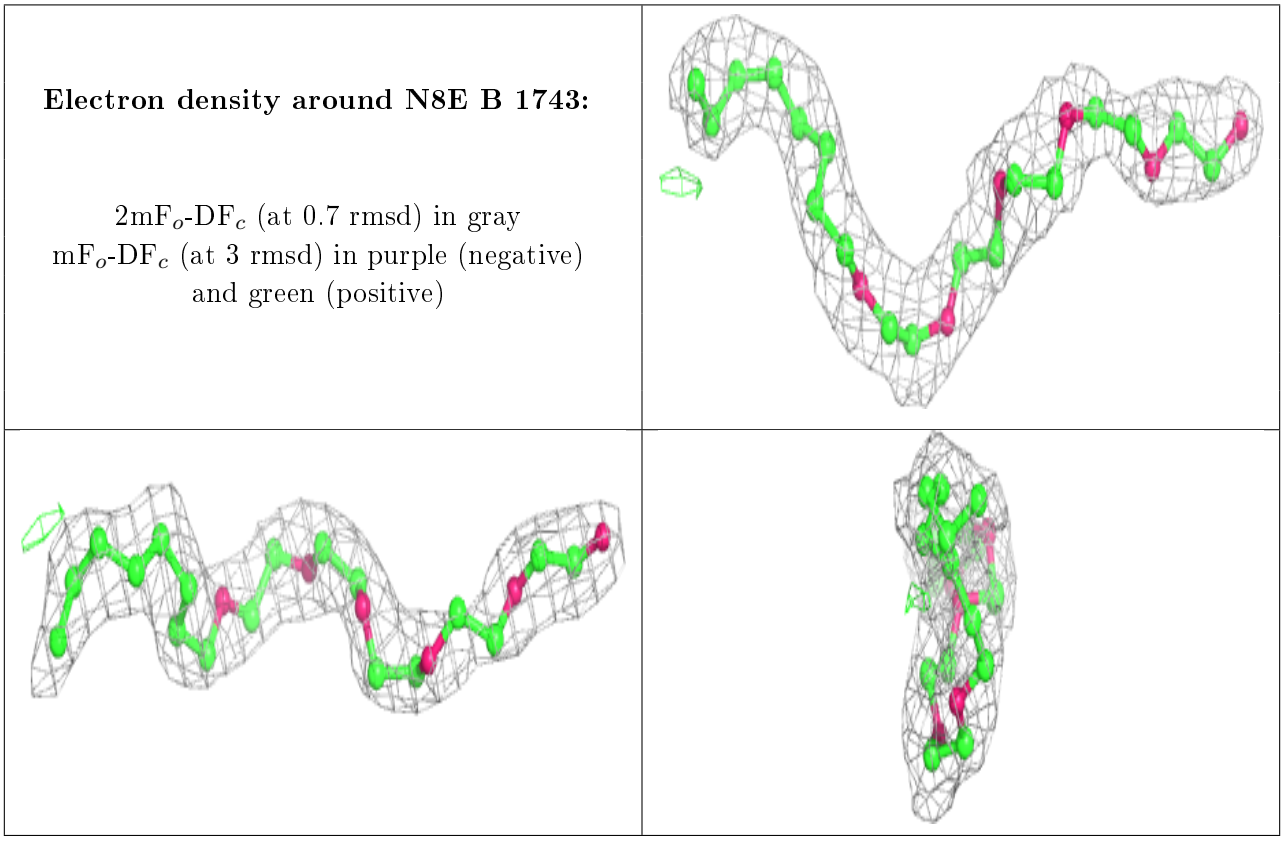
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	N8E	B	1743	24/24	0.89	0.18	12,20,35,38	0
3	N8E	A	1743	24/24	0.89	0.16	12,19,38,40	0
2	GLU	A	1744	10/10	0.93	0.21	15,20,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

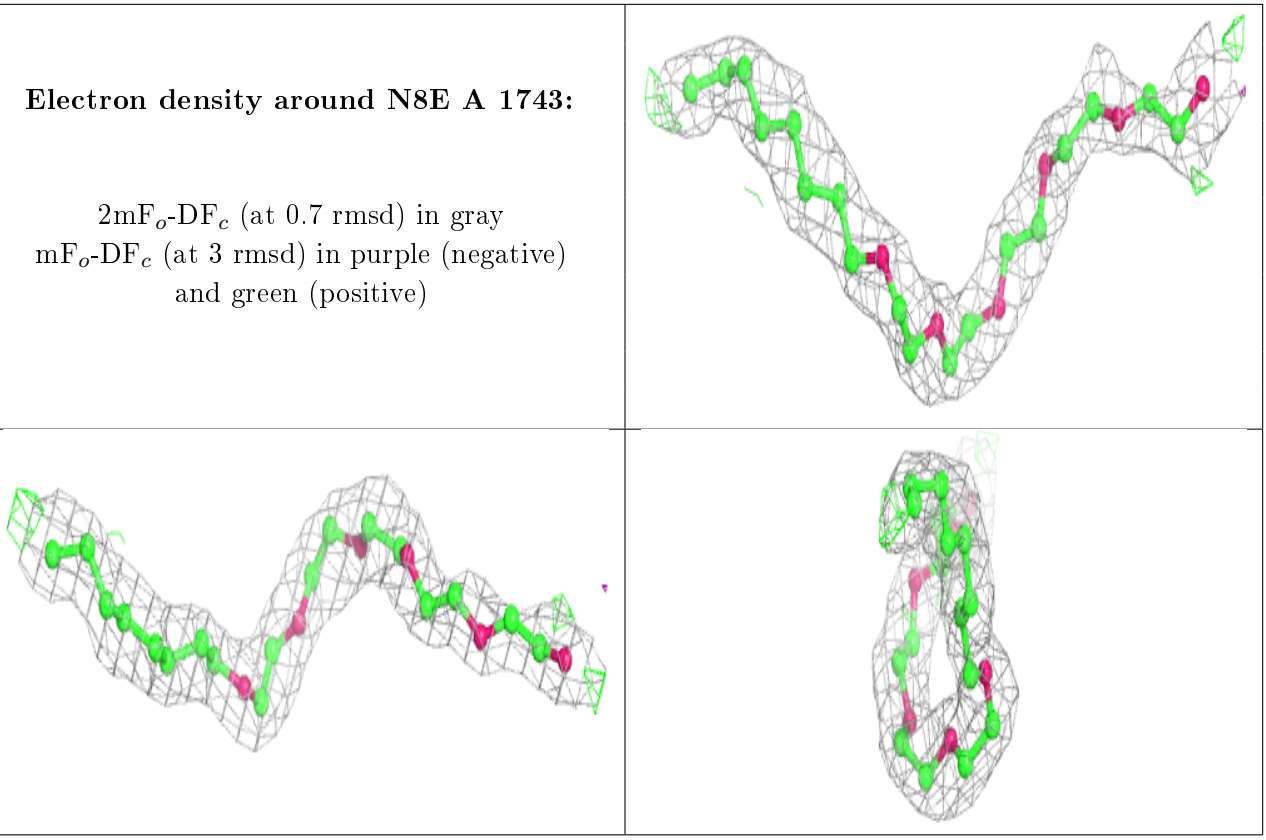
Electron density around N8E B 1743:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around N8E A 1743:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.