Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:08 am BST

PDB ID	:	2HG4
Title	:	Structure of the ketosynthase-acyltransferase didomain of module 5 from DEBS.
Authors	:	Tang, Y.; Kim, C.Y.; Mathews, I.I.; Cane, D.E.; Khosla, C.
Deposited on	:	2006-06-26
Resolution	:	2.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

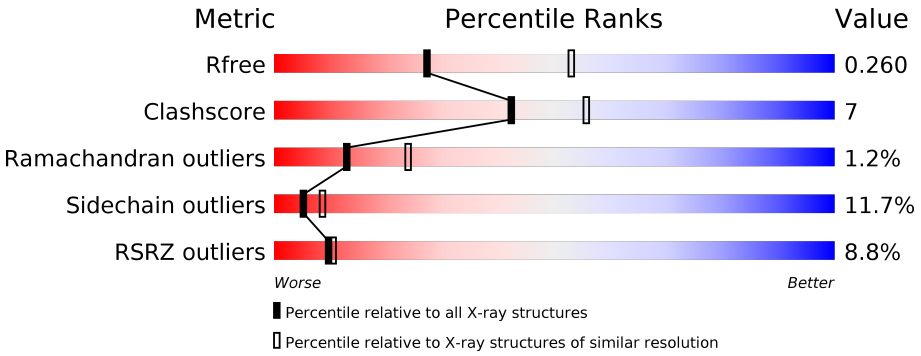
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	917	6% 76% 16%
1	B	917	8% 76% 17%
1	C	917	9% 77% 17%
1	D	917	9% 76% 18%
1	E	917	8% 79% 15%
1	F	917	9% 73% 19% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	950	-	-	X	-
2	ACT	C	950	-	-	X	-
3	SO4	C	975	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39402 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 6-Deoxyerythronolide B Synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	B	882	Total	C	N	O	S	Se	0	0	0
			6534	4054	1208	1249	8	15			
1	C	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	D	884	Total	C	N	O	S	Se	0	0	0
			6550	4064	1210	1252	8	16			
1	E	877	Total	C	N	O	S	Se	0	0	0
			6474	4016	1196	1239	8	15			
1	F	874	Total	C	N	O	S	Se	0	0	0
			6440	3995	1189	1233	8	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	525	GLU	ASP	CONFLICT	UNP Q5UNP4
A	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	732	ALA	GLY	CONFLICT	UNP Q5UNP4
A	733	HIS	ILE	CONFLICT	UNP Q5UNP4
A	734	LYS	THR	CONFLICT	UNP Q5UNP4
A	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	525	GLU	ASP	CONFLICT	UNP Q5UNP4
B	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	732	ALA	GLY	CONFLICT	UNP Q5UNP4
B	733	HIS	ILE	CONFLICT	UNP Q5UNP4
B	734	LYS	THR	CONFLICT	UNP Q5UNP4
B	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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C	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	525	GLU	ASP	CONFLICT	UNP Q5UNP4
C	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	732	ALA	GLY	CONFLICT	UNP Q5UNP4
C	733	HIS	ILE	CONFLICT	UNP Q5UNP4
C	734	LYS	THR	CONFLICT	UNP Q5UNP4
C	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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D	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	525	GLU	ASP	CONFLICT	UNP Q5UNP4
D	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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D	734	LYS	THR	CONFLICT	UNP Q5UNP4
D	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	525	GLU	ASP	CONFLICT	UNP Q5UNP4
E	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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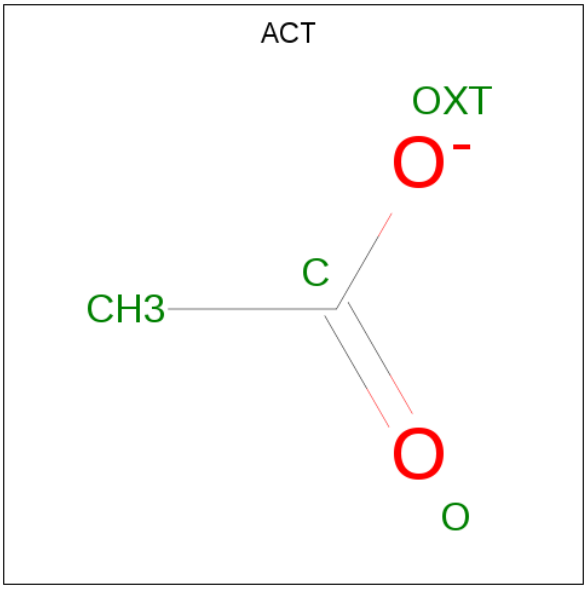
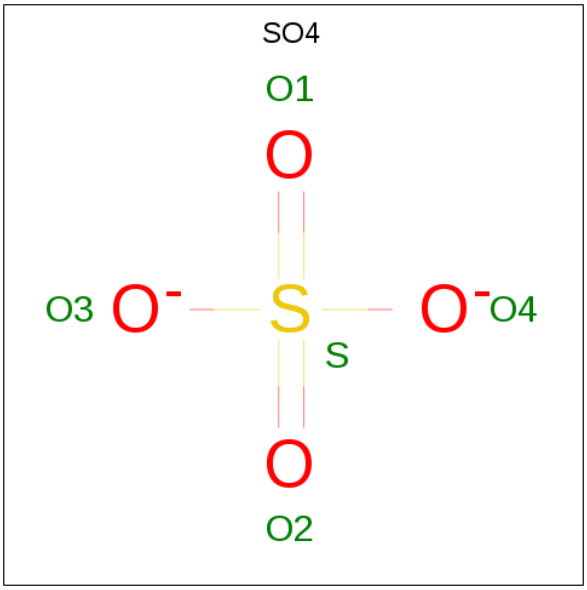
Chain	Residue	Modelled	Actual	Comment	Reference
E	732	ALA	GLY	CONFLICT	UNP Q5UNP4
E	733	HIS	ILE	CONFLICT	UNP Q5UNP4
E	734	LYS	THR	CONFLICT	UNP Q5UNP4
E	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	525	GLU	ASP	CONFLICT	UNP Q5UNP4
F	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	732	ALA	GLY	CONFLICT	UNP Q5UNP4
F	733	HIS	ILE	CONFLICT	UNP Q5UNP4
F	734	LYS	THR	CONFLICT	UNP Q5UNP4
F	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is water.

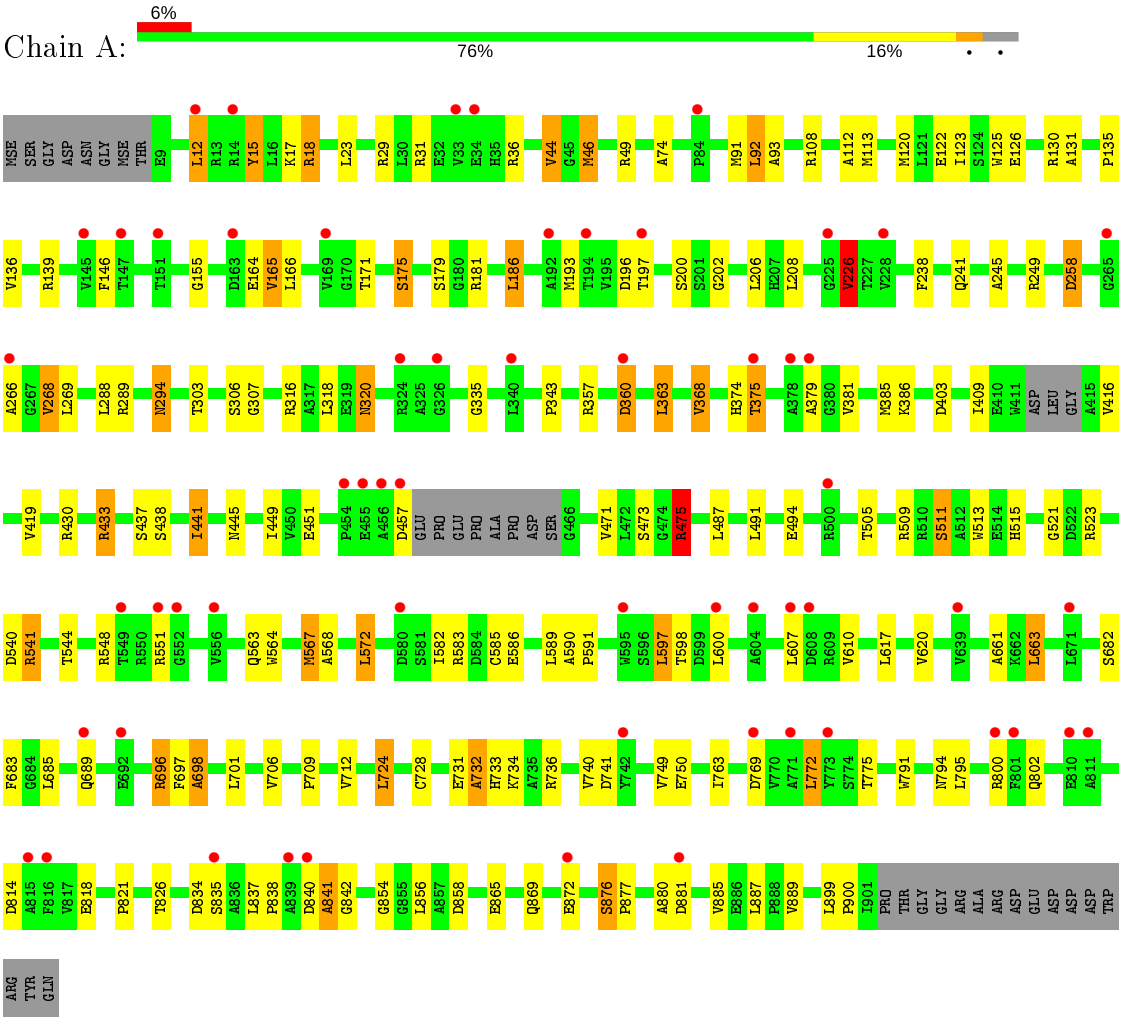
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	B	57	Total O 57 57	0	0
5	C	42	Total O 42 42	0	0
5	D	50	Total O 50 50	0	0
5	E	49	Total O 49 49	0	0
5	F	38	Total O 38 38	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

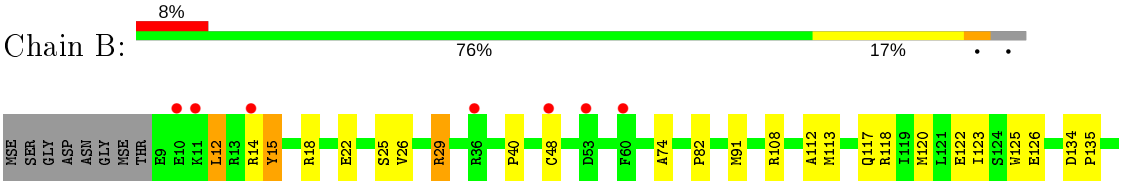
- Molecule 1: 6-Deoxyerythronolide B Synthase

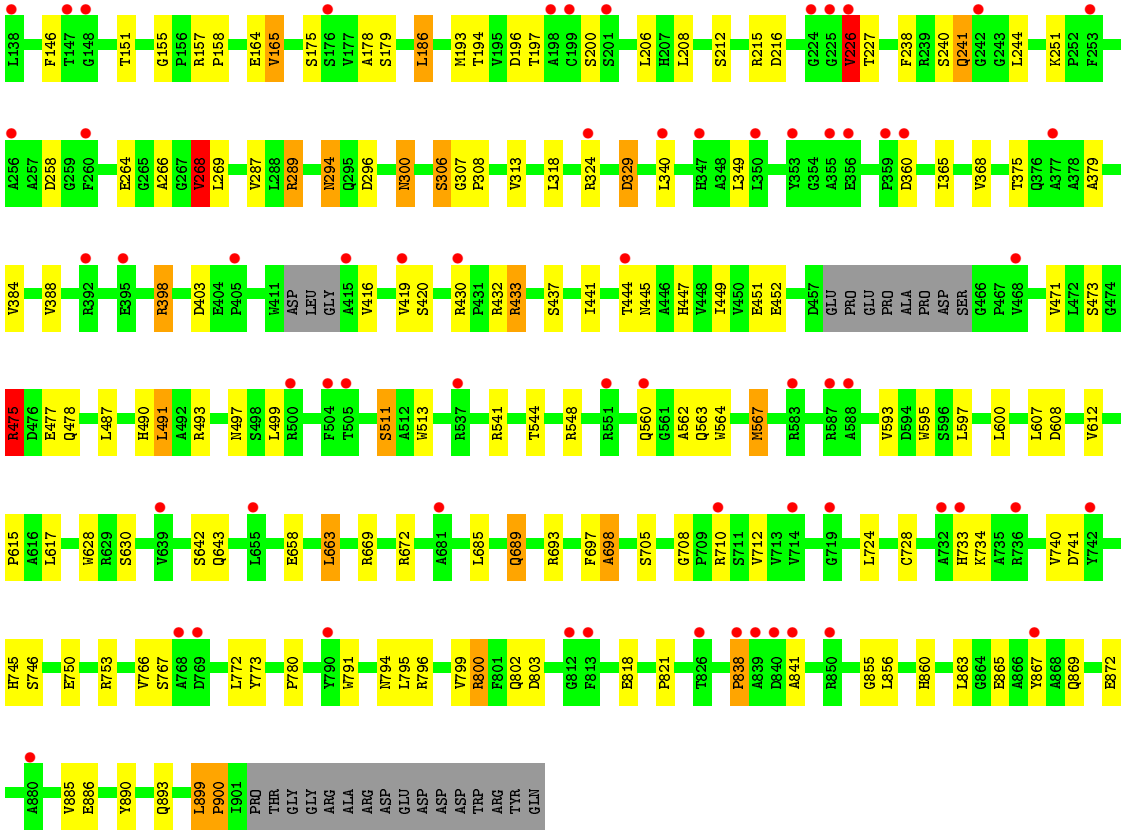
Chain A:



- Molecule 1: 6-Deoxyerythronolide B Synthase

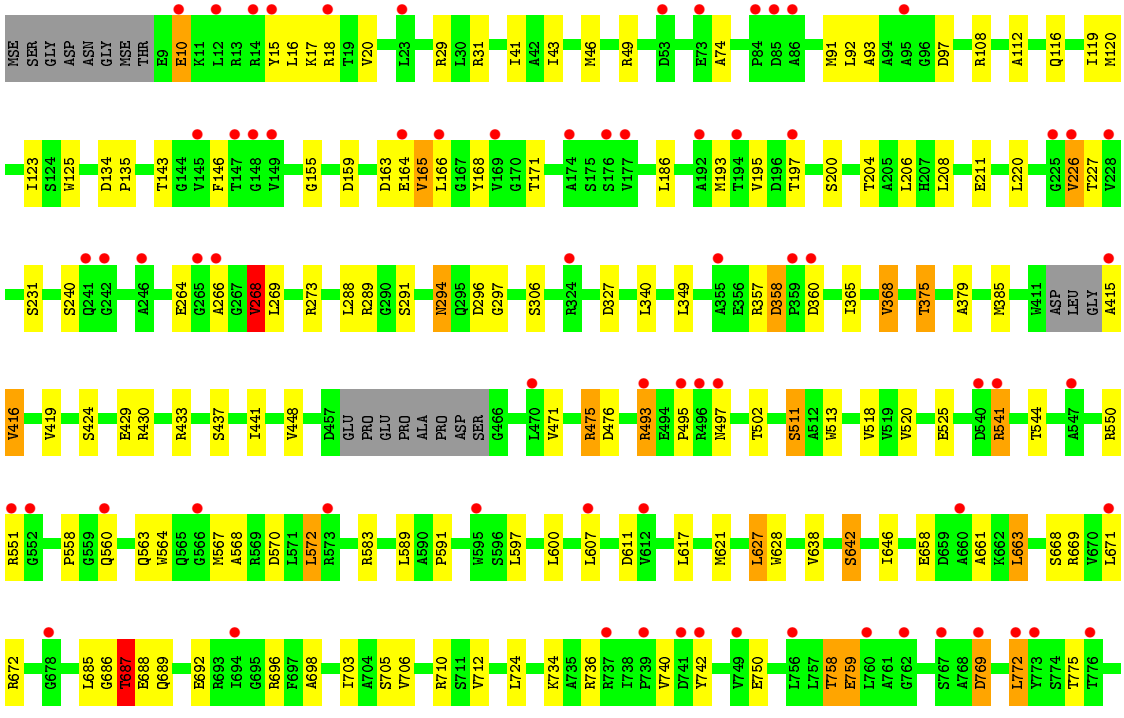
Chain B:

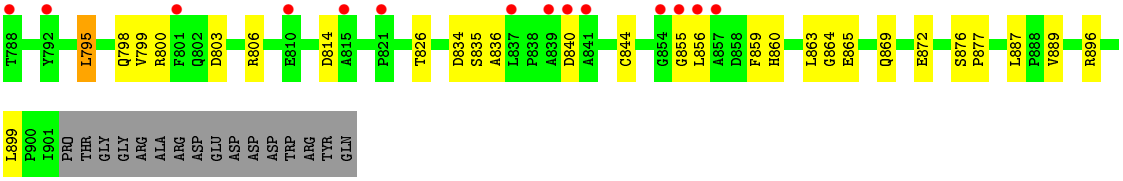




• Molecule 1: 6-Deoxyerythronolide B Synthase

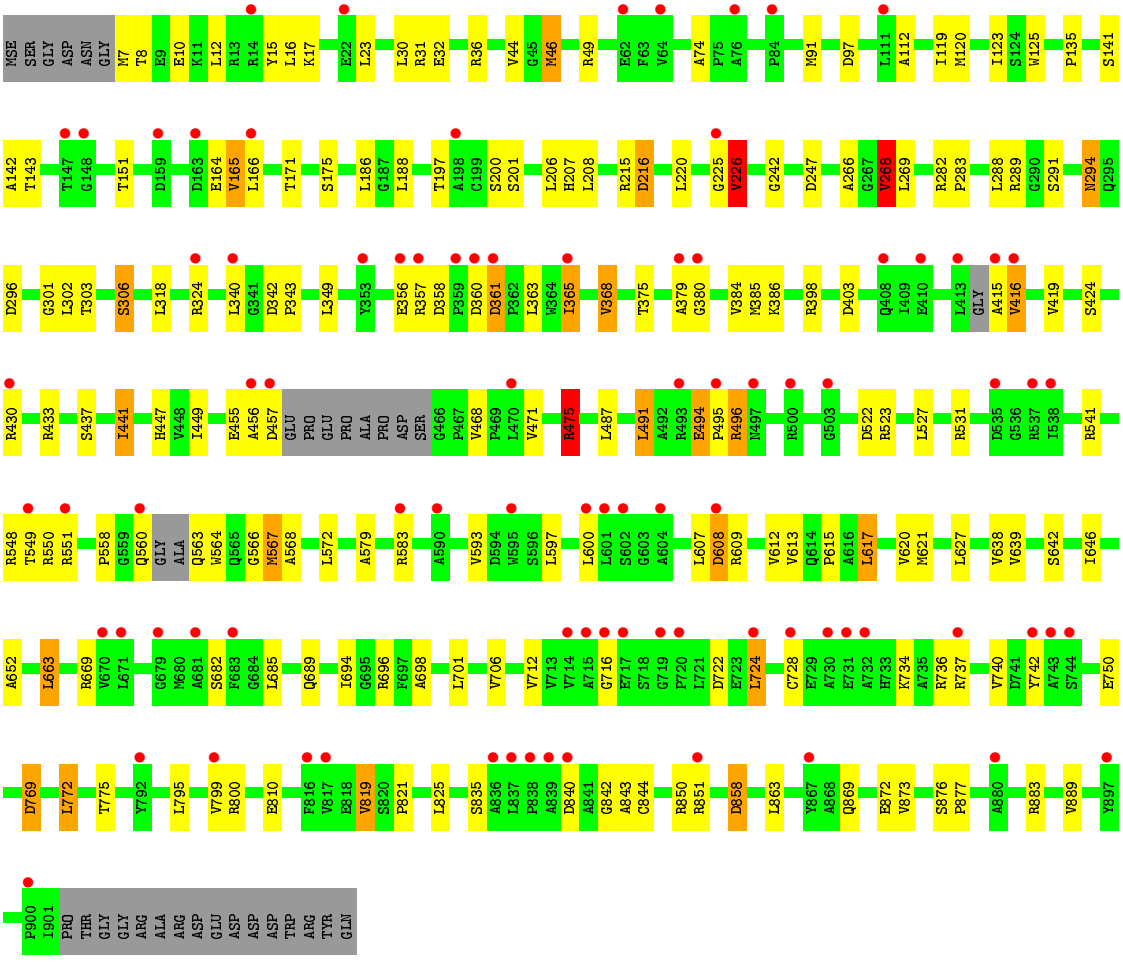
Chain C:





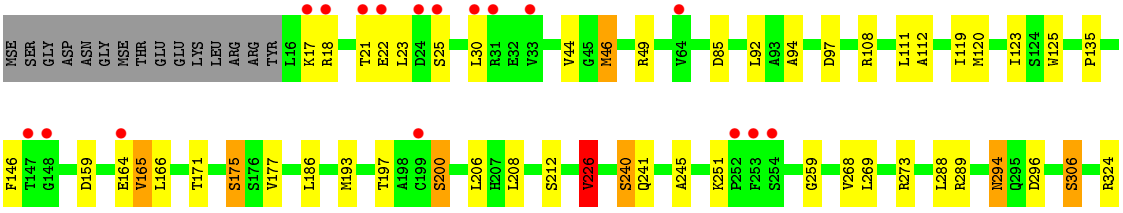
• Molecule 1: 6-Deoxyerythronolide B Synthase

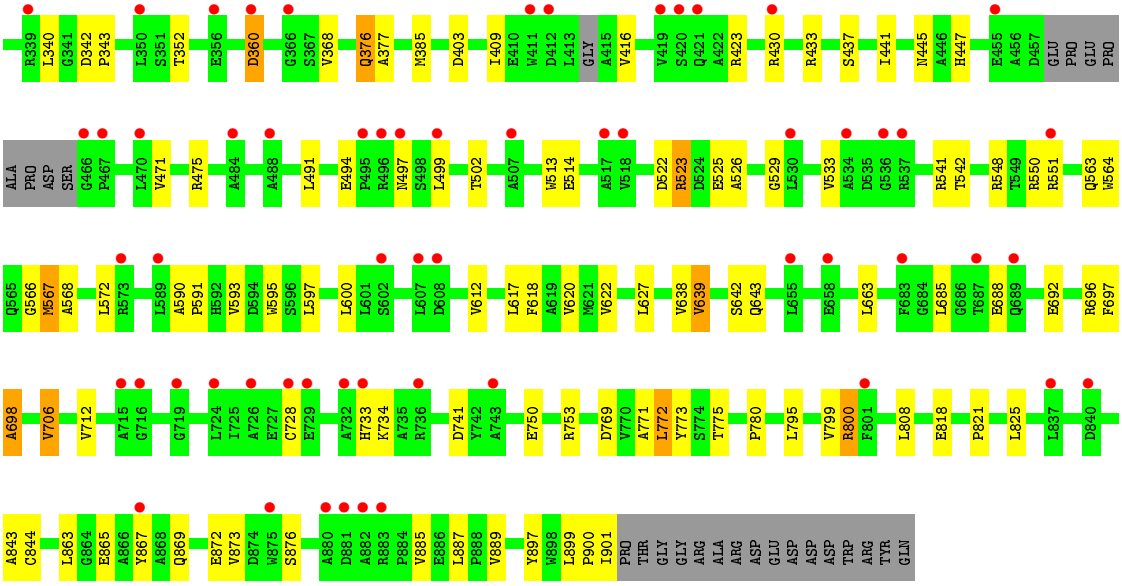
Chain D:



• Molecule 1: 6-Deoxyerythronolide B Synthase

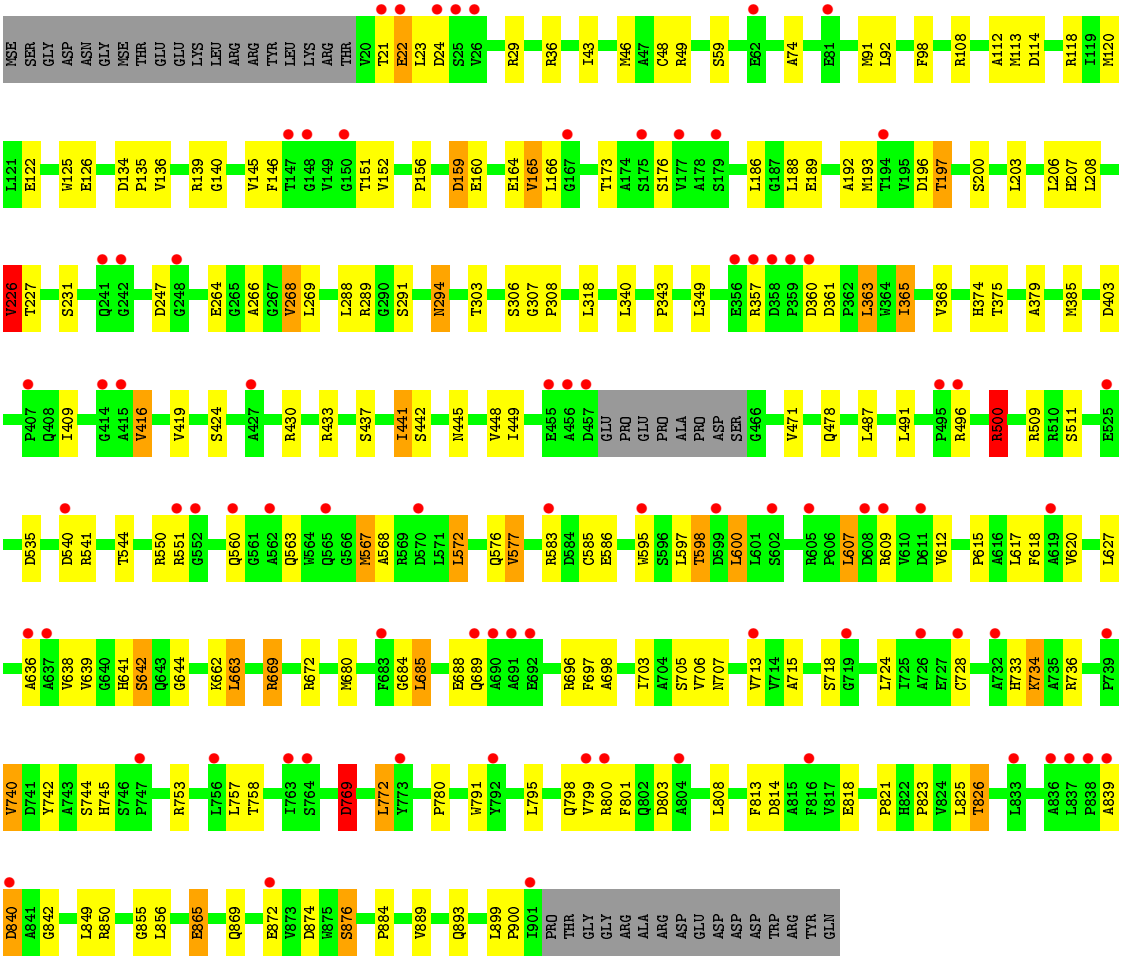
Chain E:





• Molecule 1: 6-Deoxyerythronolide B Synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	305.26Å 150.15Å 184.38Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	48.03 – 2.73 48.17 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.73) 99.8 (48.17-2.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.255 0.222 , 0.260	Depositor DCC
R_{free} test set	10395 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	39402	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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: CL, SO4, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.71	1/6634 (0.0%)	0.79	7/8999 (0.1%)
1	B	0.63	1/6648 (0.0%)	0.76	5/9015 (0.1%)
1	C	0.64	1/6634 (0.0%)	0.74	2/8999 (0.0%)
1	D	0.60	0/6663	0.73	5/9034 (0.1%)
1	E	0.58	0/6587	0.71	1/8936 (0.0%)
1	F	0.66	2/6554 (0.0%)	0.77	5/8894 (0.1%)
All	All	0.64	5/39720 (0.0%)	0.75	25/53877 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	3
1	F	0	2
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	872	GLU	CG-CD	7.16	1.62	1.51
1	B	48	CYS	CB-SG	-5.58	1.72	1.81
1	C	211	GLU	CG-CD	5.11	1.59	1.51
1	F	585	CYS	CB-SG	-5.11	1.73	1.81
1	A	585	CYS	CB-SG	-5.10	1.73	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	475	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	D	475	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	F	226	VAL	CB-CA-C	-7.03	98.05	111.40
1	A	226	VAL	CB-CA-C	-6.84	98.40	111.40
1	A	475	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	226	VAL	CB-CA-C	-6.38	99.27	111.40
1	B	475	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	E	226	VAL	CB-CA-C	-6.22	99.59	111.40
1	F	500	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	475	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	130	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	226	VAL	CB-CA-C	-5.59	100.77	111.40
1	C	368	VAL	CB-CA-C	-5.59	100.78	111.40
1	D	368	VAL	CB-CA-C	-5.53	100.90	111.40
1	F	268	VAL	CB-CA-C	-5.43	101.08	111.40
1	A	15	TYR	CA-CB-CG	-5.38	103.18	113.40
1	B	268	VAL	CB-CA-C	-5.37	101.20	111.40
1	C	268	VAL	CB-CA-C	-5.37	101.20	111.40
1	D	268	VAL	CB-CA-C	-5.35	101.23	111.40
1	F	36	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	475	ARG	CG-CD-NE	5.23	122.79	111.80
1	A	363	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	493	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	475	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	F	842	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLY	Peptide
1	A	840	ASP	Peptide
1	A	841	ALA	Peptide
1	A	842	GLY	Peptide
1	B	155	GLY	Peptide
1	C	10	GLU	Peptide
1	C	155	GLY	Peptide
1	C	840	ASP	Peptide
1	F	21	THR	Peptide
1	F	22	GLU	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	6520	0	6359	84	0
1	B	6534	0	6385	100	0
1	C	6520	0	6359	97	0
1	D	6550	0	6396	91	0
1	E	6474	0	6316	75	0
1	F	6440	0	6274	97	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
2	C	4	0	3	4	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	74	0	0	3	0
5	B	57	0	0	1	0
5	C	42	0	0	5	0
5	D	50	0	0	1	0
5	E	49	0	0	3	0
5	F	38	0	0	1	0
All	All	39402	0	38107	533	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (533) 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:B:642:SER:OG	2:B:950:ACT:O	1.71	1.06
1:F:207:HIS:HD1	1:F:291:SER:HG	1.16	0.94
1:D:617:LEU:HD22	1:D:621:MSE:HE3	1.53	0.91
1:C:193:MSE:HE3	1:C:208:LEU:HD13	1.56	0.86
1:E:564:TRP:O	1:E:567:MSE:HG3	1.78	0.84
1:A:865:GLU:O	1:A:869:GLN:HG3	1.78	0.83
1:A:193:MSE:HE3	1:A:208:LEU:HD13	1.60	0.83
1:D:294:ASN:C	1:D:294:ASN:HD22	1.81	0.81
1:D:349:LEU:HD13	1:D:365:ILE:HD11	1.62	0.80
1:F:586:GLU:OE1	1:F:598:THR:OG1	2.01	0.79
1:A:294:ASN:HD22	1:A:294:ASN:C	1.86	0.79
1:B:193:MSE:HE3	1:B:208:LEU:HD13	1.65	0.77
1:A:245:ALA:HA	1:A:258:ASP:HB2	1.64	0.77
1:F:193:MSE:HE3	1:F:208:LEU:HD13	1.69	0.74
1:F:294:ASN:HD22	1:F:294:ASN:C	1.92	0.73
1:D:701:LEU:HD23	1:D:716:GLY:HA3	1.70	0.72
1:C:294:ASN:HD22	1:C:294:ASN:C	1.94	0.72
1:D:620:VAL:HG11	1:D:821:PRO:HG3	1.71	0.72
1:A:193:MSE:CE	1:A:208:LEU:HD13	2.18	0.71
1:D:120:MSE:HE3	1:D:226:VAL:HG22	1.72	0.71
1:C:46:MSE:HB2	1:C:385:MSE:HE2	1.71	0.71
1:B:120:MSE:HE3	1:B:226:VAL:HG13	1.72	0.71
1:C:120:MSE:HE3	1:C:226:VAL:HG13	1.71	0.71
1:B:564:TRP:O	1:B:567:MSE:HG3	1.90	0.70
1:C:493:ARG:O	1:C:495:PRO:HD3	1.90	0.70
1:B:120:MSE:CE	1:B:123:ILE:HD11	2.22	0.69
1:A:136:VAL:O	1:A:139:ARG:HG3	1.92	0.69
1:C:558:PRO:HD2	1:C:621:MSE:SE	2.42	0.69
1:C:688:GLU:O	1:C:692:GLU:HG2	1.93	0.69
1:D:296:ASP:HB2	1:D:306:SER:HB3	1.75	0.69
1:D:617:LEU:CD2	1:D:621:MSE:HE3	2.23	0.69
1:B:294:ASN:HD22	1:B:294:ASN:C	1.95	0.69
1:A:320:ASN:HD22	1:A:320:ASN:N	1.88	0.69
1:B:197:THR:HG22	1:B:197:THR:O	1.93	0.68
1:B:251:LYS:NZ	1:B:258:ASP:OD2	2.28	0.67
1:E:17:LYS:O	1:E:21:THR:OG1	2.08	0.67
1:E:294:ASN:HD22	1:E:294:ASN:C	1.98	0.67
1:B:241:GLN:C	1:B:241:GLN:HE21	1.98	0.66
1:B:437:SER:HB3	1:B:447:HIS:ND1	2.11	0.66
1:E:642:SER:OG	2:E:950:ACT:C	2.43	0.66
1:A:197:THR:O	1:A:197:THR:HG22	1.94	0.65
1:A:15:TYR:CE1	1:A:18:ARG:HD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:HB2	1:B:165:VAL:HG22	1.79	0.65
1:B:193:MSE:CE	1:B:208:LEU:HD13	2.27	0.65
1:F:705:SER:CB	1:F:799:VAL:HB	2.27	0.65
1:A:206:LEU:HD21	1:A:288:LEU:HD13	1.78	0.64
1:B:146:PHE:HD1	1:B:193:MSE:HE2	1.62	0.64
1:F:206:LEU:HD21	1:F:288:LEU:HD13	1.79	0.64
1:F:728:CYS:HB3	1:F:733:HIS:HB2	1.78	0.64
1:A:112:ALA:HB2	1:A:165:VAL:HG22	1.80	0.64
1:D:724:LEU:O	1:D:728:CYS:SG	2.48	0.64
1:A:120:MSE:HE3	1:A:226:VAL:HG13	1.79	0.63
1:D:361:ASP:OD1	1:D:361:ASP:O	2.16	0.63
1:D:120:MSE:HE1	1:D:266:ALA:HB1	1.80	0.63
1:E:112:ALA:HB2	1:E:165:VAL:HG22	1.81	0.63
1:E:494:GLU:HB3	1:E:497:ASN:HD22	1.63	0.62
1:F:43:ILE:HG21	1:F:46:MSE:HE3	1.81	0.62
1:F:136:VAL:O	1:F:139:ARG:HG3	1.99	0.62
1:B:146:PHE:CD1	1:B:193:MSE:HE2	2.34	0.62
1:E:120:MSE:CE	1:E:123:ILE:HD11	2.30	0.62
1:D:475:ARG:HG3	1:D:475:ARG:HH11	1.65	0.62
1:F:206:LEU:HD23	1:F:206:LEU:C	2.20	0.61
1:B:296:ASP:HB2	1:B:306:SER:HB3	1.82	0.61
1:E:706:VAL:HG22	1:E:800:ARG:HA	1.83	0.61
1:E:566:GLY:O	1:E:568:ALA:N	2.34	0.61
1:C:206:LEU:HD21	1:C:288:LEU:HD13	1.83	0.61
1:D:638:VAL:HG23	1:D:772:LEU:HD22	1.84	0.60
1:C:193:MSE:CE	1:C:208:LEU:HD13	2.29	0.60
1:C:43:ILE:HG21	1:C:46:MSE:HE3	1.82	0.60
1:D:294:ASN:ND2	1:D:294:ASN:C	2.52	0.60
1:D:609:ARG:O	1:D:613:VAL:HG23	2.01	0.60
1:E:146:PHE:HD2	1:E:193:MSE:HE2	1.66	0.60
1:D:197:THR:O	1:D:197:THR:HG22	2.02	0.60
1:E:197:THR:HG22	1:E:197:THR:O	2.02	0.60
1:D:120:MSE:SE	1:D:226:VAL:HG22	2.52	0.60
1:F:595:TRP:CZ2	1:F:612:VAL:HA	2.35	0.60
1:F:638:VAL:HG23	1:F:772:LEU:HD22	1.84	0.60
1:A:268:VAL:O	1:A:269:LEU:HD12	2.02	0.60
1:C:296:ASP:HB2	1:C:306:SER:HB3	1.82	0.60
1:E:638:VAL:HG23	1:E:772:LEU:HD22	1.84	0.59
1:F:120:MSE:HE3	1:F:226:VAL:HG13	1.82	0.59
1:F:197:THR:CG2	1:F:197:THR:O	2.51	0.58
1:E:437:SER:HB3	1:E:447:HIS:ND1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:THR:HG22	1:E:200:SER:OG	2.02	0.58
1:E:123:ILE:HD12	1:E:268:VAL:HG23	1.86	0.58
1:D:120:MSE:HE3	1:D:226:VAL:HG13	1.85	0.58
1:F:146:PHE:HD2	1:F:193:MSE:HE2	1.68	0.58
1:A:294:ASN:ND2	1:A:294:ASN:C	2.56	0.58
1:A:564:TRP:O	1:A:567:MSE:HG3	2.03	0.58
1:C:560:GLN:NE2	1:C:742:TYR:OH	2.36	0.58
1:E:595:TRP:CZ2	1:E:612:VAL:HA	2.39	0.58
1:A:854:GLY:O	1:A:858:ASP:OD2	2.21	0.58
1:C:206:LEU:HD23	1:C:206:LEU:O	2.04	0.57
1:F:193:MSE:CE	1:F:208:LEU:HD13	2.34	0.57
1:F:471:VAL:HG12	5:F:992:HOH:O	2.03	0.57
1:B:289:ARG:HG2	1:B:289:ARG:HH11	1.69	0.57
1:C:865:GLU:O	1:C:869:GLN:HG3	2.03	0.57
1:D:120:MSE:CE	1:D:226:VAL:HG22	2.34	0.57
1:F:707:ASN:HD21	1:F:713:VAL:HG23	1.68	0.57
1:E:22:GLU:HB3	1:F:23:LEU:HD21	1.86	0.57
1:C:591:PRO:HD3	1:F:478:GLN:HE22	1.70	0.57
1:C:642:SER:OG	2:C:950:ACT:C	2.53	0.57
1:D:722:ASP:OD1	1:D:737:ARG:NH2	2.38	0.57
1:C:564:TRP:O	1:C:567:MSE:HG3	2.05	0.56
1:F:227:THR:O	1:F:264:GLU:HB2	2.04	0.56
1:F:294:ASN:ND2	1:F:445:ASN:HB2	2.19	0.56
1:F:156:PRO:HB2	1:F:160:GLU:HG3	1.87	0.56
1:B:120:MSE:HE1	1:B:123:ILE:HD11	1.86	0.56
1:D:46:MSE:CE	1:D:385:MSE:HG2	2.35	0.56
1:F:197:THR:O	1:F:197:THR:HG22	2.05	0.56
1:F:620:VAL:HG11	1:F:821:PRO:HG3	1.88	0.56
1:B:108:ARG:HD3	1:B:164:GLU:O	2.05	0.56
1:B:475:ARG:HG3	1:B:475:ARG:HH11	1.70	0.56
1:B:375:THR:HG23	1:B:379:ALA:N	2.21	0.56
1:C:799:VAL:HG22	5:C:1018:HOH:O	2.06	0.56
1:D:437:SER:HB3	1:D:447:HIS:ND1	2.20	0.56
1:B:595:TRP:CZ2	1:B:612:VAL:HA	2.41	0.56
1:C:120:MSE:HE1	1:C:123:ILE:HD11	1.88	0.56
1:B:773:TYR:HA	1:B:780:PRO:HA	1.88	0.55
1:B:289:ARG:HG2	1:B:289:ARG:NH1	2.19	0.55
1:C:197:THR:O	1:C:197:THR:HG22	2.06	0.55
1:D:197:THR:HG22	1:D:200:SER:OG	2.06	0.55
1:D:32:GLU:OE1	1:D:36:ARG:CZ	2.54	0.55
1:E:901:ILE:C	5:E:1002:HOH:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MSE:HE1	1:D:15:TYR:CE2	2.42	0.55
1:F:146:PHE:CD2	1:F:193:MSE:HE2	2.42	0.55
1:B:113:MSE:HE2	1:B:118:ARG:HG2	1.89	0.55
1:F:705:SER:HB2	1:F:799:VAL:HB	1.88	0.55
1:B:766:VAL:HG12	1:B:767:SER:O	2.06	0.55
1:D:375:THR:HG23	1:D:379:ALA:N	2.22	0.54
1:B:499:LEU:N	3:B:975:SO4:O1	2.31	0.54
1:E:146:PHE:CD2	1:E:193:MSE:HE2	2.43	0.54
1:B:12:LEU:HD12	1:B:15:TYR:HD2	1.72	0.54
1:F:120:MSE:HE1	1:F:266:ALA:HB1	1.89	0.54
1:C:108:ARG:HD2	1:C:168:TYR:HE2	1.70	0.54
1:D:215:ARG:O	1:D:216:ASP:HB2	2.07	0.54
1:E:728:CYS:HB3	1:E:733:HIS:HB2	1.89	0.54
1:C:876:SER:HB2	1:C:877:PRO:HD3	1.90	0.54
1:D:858:ASP:OD1	1:D:858:ASP:N	2.40	0.54
1:E:523:ARG:O	1:E:526:ALA:HB3	2.08	0.54
1:C:15:TYR:HE2	1:E:551:ARG:CZ	2.21	0.54
1:D:769:ASP:N	1:D:769:ASP:OD1	2.30	0.53
1:B:728:CYS:HB3	1:B:733:HIS:HB2	1.90	0.53
1:A:74:ALA:HA	1:A:91:MSE:HG3	1.91	0.53
1:F:821:PRO:HA	1:F:849:LEU:HB2	1.90	0.53
1:C:195:VAL:HG21	1:C:208:LEU:HD12	1.90	0.53
1:C:227:THR:O	1:C:264:GLU:HB2	2.09	0.53
1:F:294:ASN:ND2	1:F:294:ASN:C	2.59	0.53
1:D:455:GLU:HA	1:D:455:GLU:OE1	2.08	0.53
1:A:197:THR:O	1:A:197:THR:CG2	2.56	0.53
1:D:775:THR:O	1:D:799:VAL:O	2.27	0.52
1:C:15:TYR:CE2	1:E:551:ARG:CZ	2.93	0.52
1:C:710:ARG:CG	1:C:710:ARG:O	2.56	0.52
1:D:527:LEU:O	1:D:531:ARG:HG3	2.09	0.52
1:F:349:LEU:HD13	1:F:365:ILE:HD11	1.90	0.52
1:B:433:ARG:NH1	1:B:451:GLU:OE1	2.42	0.52
1:C:475:ARG:HD3	1:C:513:TRP:CD2	2.44	0.52
1:B:113:MSE:HE2	1:B:118:ARG:CG	2.40	0.52
1:B:25:SER:O	1:B:29:ARG:HB2	2.09	0.52
1:C:415:ALA:HB1	5:C:1006:HOH:O	2.08	0.52
1:E:620:VAL:HG11	1:E:821:PRO:HG3	1.92	0.52
1:A:343:PRO:HA	1:A:409:ILE:HG12	1.91	0.52
1:C:358:ASP:N	1:C:358:ASP:OD1	2.43	0.52
1:B:669:ARG:HG2	1:B:672:ARG:HH12	1.75	0.52
1:A:433:ARG:NH1	1:A:451:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:O	1:B:216:ASP:HB2	2.09	0.52
1:F:874:ASP:OD1	1:F:876:SER:OG	2.19	0.52
1:A:294:ASN:ND2	1:A:445:ASN:HB2	2.26	0.51
1:A:505:THR:HB	1:A:887:LEU:HD11	1.92	0.51
1:C:646:ILE:HG12	1:C:663:LEU:HD13	1.91	0.51
1:D:120:MSE:CE	1:D:266:ALA:HB1	2.40	0.51
1:F:576:GLN:O	1:F:577:VAL:C	2.49	0.51
1:E:865:GLU:O	1:E:869:GLN:HG3	2.10	0.51
1:F:639:VAL:CG2	1:F:808:LEU:HD11	2.40	0.51
1:D:642:SER:OG	2:D:950:ACT:C	2.59	0.51
1:C:268:VAL:C	1:C:269:LEU:HD12	2.31	0.51
1:E:108:ARG:HD3	1:E:164:GLU:O	2.11	0.51
1:A:521:GLY:HA2	5:A:1000:HOH:O	2.10	0.51
1:C:710:ARG:HG2	1:C:710:ARG:O	2.11	0.51
1:D:560:GLN:NE2	1:D:742:TYR:OH	2.40	0.51
1:B:123:ILE:HD12	1:B:268:VAL:CG2	2.41	0.51
1:C:638:VAL:HG23	1:C:772:LEU:HD22	1.92	0.51
1:E:818:GLU:OE2	1:E:825:LEU:N	2.39	0.51
1:C:116:GLN:O	1:C:120:MSE:HG2	2.11	0.51
1:E:197:THR:O	1:E:197:THR:CG2	2.59	0.51
1:E:22:GLU:HA	1:E:25:SER:OG	2.11	0.51
1:A:113:MSE:HE3	1:A:181:ARG:NE	2.26	0.50
1:A:316:ARG:O	1:A:320:ASN:ND2	2.45	0.50
1:E:688:GLU:OE1	1:E:688:GLU:N	2.44	0.50
1:C:197:THR:O	1:C:197:THR:CG2	2.59	0.50
1:F:684:GLY:HA3	1:F:734:LYS:HB2	1.93	0.50
1:C:273:ARG:HB2	5:C:1009:HOH:O	2.10	0.50
1:D:456:ALA:O	1:D:457:ASP:HB3	2.12	0.50
1:A:268:VAL:C	1:A:269:LEU:HD12	2.31	0.50
1:B:122:GLU:O	1:B:126:GLU:HG3	2.11	0.50
1:D:120:MSE:HE3	1:D:226:VAL:CG2	2.40	0.50
1:B:22:GLU:O	1:B:26:VAL:HG23	2.12	0.50
1:B:294:ASN:ND2	1:B:294:ASN:C	2.64	0.50
1:B:74:ALA:HA	1:B:91:MSE:HG3	1.92	0.50
1:B:865:GLU:O	1:B:869:GLN:HG3	2.12	0.50
1:C:502:THR:HG23	1:C:887:LEU:HD21	1.94	0.50
1:E:120:MSE:HE1	1:E:123:ILE:HD11	1.93	0.50
1:C:208:LEU:HD22	1:D:208:LEU:HD22	1.94	0.50
1:F:120:MSE:CE	1:F:266:ALA:HB1	2.41	0.50
1:B:186:LEU:N	1:B:186:LEU:HD23	2.26	0.50
1:F:703:ILE:O	1:F:798:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:N	1:B:452:GLU:OE1	2.33	0.49
1:C:705:SER:CB	1:C:799:VAL:HB	2.42	0.49
1:E:590:ALA:N	1:E:591:PRO:HD2	2.26	0.49
1:F:303:THR:HA	1:F:441:ILE:O	2.12	0.49
1:B:12:LEU:HD12	1:B:15:TYR:CD2	2.46	0.49
1:C:146:PHE:HD2	1:C:193:MSE:HE2	1.77	0.49
1:C:74:ALA:HA	1:C:91:MSE:HG3	1.94	0.49
1:F:636:ALA:HB3	1:F:813:PHE:HE1	1.78	0.49
1:F:769:ASP:N	1:F:769:ASP:OD1	2.45	0.49
1:A:112:ALA:HB2	1:A:165:VAL:CG2	2.42	0.49
1:B:238:PHE:O	1:B:241:GLN:O	2.29	0.49
1:B:329:ASP:OD1	1:B:329:ASP:N	2.44	0.49
1:D:112:ALA:HB2	1:D:165:VAL:HG22	1.94	0.49
1:F:112:ALA:HB2	1:F:165:VAL:HG22	1.94	0.49
1:F:680:MSE:HE3	1:F:715:ALA:HB2	1.95	0.49
1:C:119:ILE:O	1:C:123:ILE:HG12	2.12	0.49
1:D:358:ASP:OD2	1:D:360:ASP:HB3	2.13	0.49
1:F:500:ARG:HH11	1:F:500:ARG:HB3	1.78	0.49
1:F:74:ALA:HA	1:F:91:MSE:HG3	1.93	0.49
1:B:398:ARG:CG	1:B:420:SER:O	2.61	0.49
1:A:108:ARG:HD3	1:A:164:GLU:O	2.12	0.49
1:C:856:LEU:HD22	1:C:860:HIS:CE1	2.48	0.49
1:E:773:TYR:HA	1:E:780:PRO:HA	1.95	0.49
1:B:318:LEU:HD23	1:B:449:ILE:HD13	1.96	0.48
1:D:646:ILE:HG12	1:D:663:LEU:HD13	1.94	0.48
1:A:709:PRO:N	1:A:802:GLN:HE22	2.11	0.48
1:B:120:MSE:HE2	1:B:123:ILE:HD11	1.94	0.48
1:A:238:PHE:O	1:A:241:GLN:O	2.32	0.48
1:E:294:ASN:ND2	1:E:294:ASN:C	2.66	0.48
1:B:197:THR:CG2	1:B:197:THR:O	2.60	0.48
1:C:814:ASP:N	1:C:814:ASP:OD1	2.45	0.48
1:D:386:LYS:NZ	5:D:1001:HOH:O	2.39	0.48
1:B:125:TRP:CE2	1:B:135:PRO:HG2	2.49	0.48
1:C:627:LEU:HD22	1:C:859:PHE:CE2	2.49	0.48
1:C:611:ASP:HA	1:C:668:SER:HB2	1.94	0.48
1:D:357:ARG:HB2	1:D:415:ALA:HB2	1.95	0.48
1:E:120:MSE:HE3	1:E:226:VAL:HG13	1.95	0.48
1:E:245:ALA:HB2	1:E:259:GLY:O	2.13	0.48
1:C:294:ASN:ND2	1:C:294:ASN:C	2.66	0.48
1:C:703:ILE:O	1:C:798:GLN:HG3	2.14	0.48
1:E:193:MSE:CE	1:E:208:LEU:HD13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLY:HA3	5:A:1037:HOH:O	2.14	0.48
1:C:365:ILE:HD12	1:C:416:VAL:HG13	1.94	0.48
1:D:579:ALA:HB1	1:D:583:ARG:NH2	2.29	0.48
1:B:697:PHE:O	1:B:698:ALA:C	2.51	0.48
1:E:775:THR:O	1:E:799:VAL:O	2.31	0.48
1:F:568:ALA:O	1:F:572:LEU:HB2	2.14	0.48
1:A:375:THR:HG23	1:A:379:ALA:N	2.29	0.48
1:C:146:PHE:CD2	1:C:193:MSE:HE2	2.49	0.48
1:F:728:CYS:O	1:F:733:HIS:N	2.39	0.48
1:F:108:ARG:HD3	1:F:164:GLU:O	2.14	0.48
1:F:343:PRO:HA	1:F:409:ILE:HG12	1.96	0.48
1:E:206:LEU:HD21	1:E:288:LEU:HD13	1.95	0.47
1:E:296:ASP:HB2	1:E:306:SER:HB3	1.95	0.47
1:A:146:PHE:HD2	1:A:193:MSE:HE2	1.80	0.47
1:B:197:THR:HG23	1:B:444:THR:HB	1.96	0.47
1:A:186:LEU:N	1:A:186:LEU:HD23	2.29	0.47
1:A:589:LEU:HD23	1:A:661:ALA:HB1	1.96	0.47
1:D:7:MSE:HE1	1:D:15:TYR:CD2	2.49	0.47
1:B:475:ARG:HH11	1:B:475:ARG:CG	2.27	0.47
1:A:568:ALA:O	1:A:572:LEU:HB2	2.15	0.47
1:A:876:SER:N	1:A:877:PRO:CD	2.77	0.47
1:B:471:VAL:CG2	1:B:867:TYR:CE2	2.97	0.47
1:B:562:ALA:HB1	1:B:821:PRO:HD2	1.97	0.47
1:F:663:LEU:HD11	1:F:791:TRP:CE2	2.50	0.47
1:A:197:THR:HG22	1:A:200:SER:OG	2.14	0.47
1:A:728:CYS:HB3	1:A:733:HIS:HB2	1.96	0.47
1:D:365:ILE:HD12	1:D:416:VAL:HG13	1.95	0.47
1:E:240:SER:C	1:E:241:GLN:O	2.50	0.47
1:C:206:LEU:HD23	1:C:206:LEU:C	2.35	0.47
1:E:566:GLY:O	1:E:567:MSE:C	2.51	0.47
1:F:375:THR:HG23	1:F:379:ALA:N	2.29	0.47
1:B:642:SER:OG	1:B:643:GLN:N	2.46	0.47
1:B:745:HIS:HA	1:B:796:ARG:O	2.14	0.47
1:C:627:LEU:HD22	1:C:859:PHE:CZ	2.50	0.47
1:B:384:VAL:O	1:B:388:VAL:HG23	2.15	0.47
1:C:120:MSE:HE1	1:C:266:ALA:HB1	1.96	0.47
1:E:46:MSE:CE	1:E:385:MSE:HG2	2.45	0.47
1:A:196:ASP:OD2	1:B:175:SER:HB3	2.15	0.47
1:E:771:ALA:HA	5:E:987:HOH:O	2.14	0.47
1:F:197:THR:CG2	1:F:200:SER:OG	2.63	0.47
1:F:697:PHE:O	1:F:698:ALA:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:VAL:HB	1:C:541:ARG:HB3	1.97	0.46
1:C:560:GLN:HE21	2:C:950:ACT:C	2.28	0.46
1:A:320:ASN:ND2	1:A:320:ASN:N	2.60	0.46
1:A:475:ARG:HH11	1:A:475:ARG:HG3	1.79	0.46
1:B:560:GLN:NE2	1:B:643:GLN:HE22	2.13	0.46
1:C:476:ASP:OD1	1:C:476:ASP:C	2.54	0.46
1:F:839:ALA:O	1:F:840:ASP:CB	2.63	0.46
1:A:12:LEU:N	1:A:12:LEU:HD23	2.31	0.46
1:D:863:LEU:HD22	1:D:873:VAL:CG1	2.45	0.46
1:A:586:GLU:OE1	1:A:598:THR:OG1	2.26	0.46
1:E:193:MSE:HE3	1:E:208:LEU:HD13	1.97	0.46
1:F:206:LEU:HD23	1:F:206:LEU:O	2.16	0.46
1:C:193:MSE:HE1	1:D:208:LEU:HD21	1.98	0.46
1:E:119:ILE:O	1:E:123:ILE:HG12	2.16	0.46
1:E:123:ILE:CD1	1:E:268:VAL:HG23	2.46	0.46
1:B:642:SER:OG	2:B:950:ACT:C	2.58	0.46
1:B:710:ARG:O	1:B:710:ARG:HG2	2.15	0.46
1:E:343:PRO:HA	1:E:409:ILE:HG12	1.98	0.46
1:D:207:HIS:ND1	1:D:291:SER:OG	2.48	0.46
1:D:567:MSE:O	1:D:568:ALA:HB3	2.15	0.46
1:E:125:TRP:CE2	1:E:135:PRO:HG2	2.51	0.46
1:F:114:ASP:OD2	1:F:152:VAL:HG13	2.15	0.46
1:A:303:THR:HA	1:A:441:ILE:O	2.16	0.45
1:B:120:MSE:CE	1:B:266:ALA:HB1	2.46	0.45
1:D:363:LEU:O	1:D:416:VAL:HA	2.16	0.45
1:A:697:PHE:O	1:A:698:ALA:C	2.54	0.45
1:B:175:SER:OG	1:B:194:THR:HG21	2.16	0.45
1:B:349:LEU:HD13	1:B:365:ILE:HD11	1.98	0.45
1:C:268:VAL:O	1:C:269:LEU:HD12	2.16	0.45
1:D:566:GLY:O	1:D:567:MSE:O	2.34	0.45
1:F:140:GLY:HA2	1:F:189:GLU:OE2	2.16	0.45
1:F:839:ALA:O	1:F:840:ASP:HB2	2.16	0.45
1:B:241:GLN:HE21	1:B:241:GLN:CA	2.28	0.45
1:D:475:ARG:CG	1:D:475:ARG:HH11	2.27	0.45
1:F:740:VAL:HG22	1:F:742:TYR:CE1	2.50	0.45
1:F:560:GLN:HG2	2:F:950:ACT:H1	1.97	0.45
1:B:82:PRO:HA	5:B:997:HOH:O	2.16	0.45
1:C:518:VAL:HG21	1:C:864:GLY:HA2	1.98	0.45
1:E:502:THR:HG23	1:E:887:LEU:HD21	1.98	0.45
1:A:772:LEU:HD12	1:A:772:LEU:C	2.37	0.45
1:D:120:MSE:CE	1:D:123:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:MSE:SE	1:E:226:VAL:HG22	2.66	0.45
1:F:186:LEU:HB2	1:F:188:LEU:HG	1.99	0.45
1:F:753:ARG:HG2	1:F:757:LEU:HD12	1.98	0.45
1:F:478:GLN:HG2	1:F:893:GLN:OE1	2.16	0.45
1:A:165:VAL:HG13	1:A:165:VAL:O	2.17	0.45
1:A:567:MSE:O	1:A:568:ALA:HB3	2.17	0.45
1:B:117:GLN:HG2	1:B:178:ALA:HA	1.99	0.45
1:D:608:ASP:OD1	1:D:608:ASP:N	2.49	0.45
1:E:186:LEU:HD23	1:E:186:LEU:N	2.31	0.45
1:B:197:THR:HG22	1:B:200:SER:OG	2.17	0.45
1:B:838:PRO:HB2	1:B:841:ALA:HB3	1.99	0.45
1:A:146:PHE:CD2	1:A:193:MSE:HE2	2.52	0.45
1:B:300:ASN:ND2	1:B:300:ASN:H	2.14	0.45
1:D:225:GLY:O	1:D:266:ALA:HA	2.17	0.45
1:B:705:SER:CB	1:B:799:VAL:HB	2.46	0.45
1:F:801:PHE:CZ	1:F:825:LEU:HD13	2.52	0.45
1:A:381:VAL:O	1:A:385:MSE:HG3	2.17	0.44
1:C:686:GLY:O	1:C:687:THR:C	2.55	0.44
1:E:342:ASP:HB2	1:E:343:PRO:HD3	1.99	0.44
1:C:123:ILE:HD12	1:C:268:VAL:HG23	1.98	0.44
1:C:705:SER:HA	1:C:799:VAL:HB	1.99	0.44
1:E:111:LEU:HA	1:E:897:TYR:HB3	2.00	0.44
1:F:641:HIS:O	1:F:644:GLY:N	2.49	0.44
1:B:294:ASN:ND2	1:B:445:ASN:HB2	2.32	0.44
1:C:197:THR:HG21	1:C:204:THR:OG1	2.18	0.44
1:D:119:ILE:O	1:D:123:ILE:HG12	2.17	0.44
1:D:301:GLY:O	1:D:302:LEU:C	2.55	0.44
1:E:268:VAL:O	1:E:269:LEU:HD12	2.17	0.44
1:E:475:ARG:HD2	1:E:513:TRP:CD2	2.52	0.44
1:F:98:PHE:CD1	1:F:118:ARG:HB3	2.52	0.44
1:C:125:TRP:CE2	1:C:135:PRO:HG2	2.52	0.44
1:E:177:VAL:HG22	1:F:442:SER:HB3	1.99	0.44
1:E:475:ARG:HD2	1:E:513:TRP:CE3	2.53	0.44
1:E:618:PHE:O	1:E:622:VAL:HG23	2.17	0.44
1:A:368:VAL:HG13	1:A:386:LYS:HD2	1.99	0.44
1:A:731:GLU:O	1:A:732:ALA:HB3	2.17	0.44
1:B:268:VAL:O	1:B:269:LEU:HD12	2.18	0.44
1:B:669:ARG:HG2	1:B:672:ARG:NH1	2.32	0.44
1:C:163:ASP:CB	1:C:166:LEU:HD12	2.48	0.44
1:D:268:VAL:O	1:D:269:LEU:HD12	2.18	0.44
1:D:206:LEU:HD21	1:D:288:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:VAL:O	1:D:615:PRO:HD2	2.18	0.44
1:F:122:GLU:O	1:F:126:GLU:HG3	2.16	0.44
1:A:46:MSE:CE	1:A:269:LEU:HD11	2.48	0.44
1:B:398:ARG:HG3	1:B:420:SER:O	2.16	0.44
1:D:74:ALA:HA	1:D:91:MSE:HG3	1.99	0.44
1:E:94:ALA:HB1	1:E:97:ASP:CG	2.38	0.44
1:A:318:LEU:HD23	1:A:449:ILE:HD13	2.00	0.44
1:C:686:GLY:O	1:C:688:GLU:N	2.51	0.44
1:D:564:TRP:O	1:D:567:MSE:HG2	2.18	0.44
1:B:856:LEU:HD22	1:B:860:HIS:CE1	2.52	0.44
1:C:799:VAL:HG13	5:C:1018:HOH:O	2.17	0.44
1:A:475:ARG:HD2	1:A:513:TRP:CD2	2.53	0.43
1:B:478:GLN:NE2	1:B:893:GLN:OE1	2.50	0.43
1:D:522:ASP:C	1:D:522:ASP:OD1	2.56	0.43
1:E:294:ASN:ND2	1:E:445:ASN:HB2	2.33	0.43
1:E:175:SER:HB3	1:F:196:ASP:OD2	2.17	0.43
1:F:294:ASN:HD21	1:F:445:ASN:HB2	1.83	0.43
1:A:120:MSE:HE1	1:A:266:ALA:HB1	2.00	0.43
1:A:123:ILE:HD12	1:A:268:VAL:HG23	2.00	0.43
1:A:375:THR:HG22	1:A:379:ALA:HA	2.00	0.43
1:A:44:VAL:HG13	1:A:131:ALA:HB1	2.00	0.43
1:B:238:PHE:HA	1:B:241:GLN:HE22	1.83	0.43
1:C:375:THR:HG23	1:C:379:ALA:N	2.33	0.43
1:A:663:LEU:HD11	1:A:791:TRP:CE2	2.53	0.43
1:C:120:MSE:HE3	1:C:226:VAL:CG1	2.43	0.43
1:A:125:TRP:CE2	1:A:135:PRO:HG2	2.53	0.43
1:D:380:GLY:O	1:D:384:VAL:HG23	2.18	0.43
1:F:567:MSE:O	1:F:568:ALA:HB3	2.17	0.43
1:A:511:SER:HB2	1:A:513:TRP:CE2	2.53	0.43
1:B:612:VAL:O	1:B:615:PRO:HD2	2.18	0.43
1:C:511:SER:HB2	1:C:513:TRP:CE2	2.53	0.43
1:D:494:GLU:OE1	1:D:494:GLU:HA	2.17	0.43
1:E:165:VAL:HG11	1:E:899:LEU:HD11	2.01	0.43
1:E:268:VAL:C	1:E:269:LEU:HD12	2.39	0.43
1:F:639:VAL:HG21	1:F:808:LEU:HD11	1.99	0.43
1:D:151:THR:O	1:D:151:THR:HG23	2.19	0.43
1:D:282:ARG:HB3	1:D:283:PRO:HD2	2.00	0.43
1:A:46:MSE:HE3	1:A:269:LEU:HG	2.01	0.43
1:B:689:GLN:HE22	1:B:693:ARG:NH1	2.16	0.43
1:D:200:SER:O	1:D:201:SER:C	2.56	0.43
1:F:46:MSE:HE2	1:F:269:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:641:HIS:O	1:F:642:SER:C	2.57	0.43
1:F:865:GLU:O	1:F:869:GLN:HG3	2.18	0.43
1:A:728:CYS:O	1:A:732:ALA:N	2.52	0.43
1:D:10:GLU:N	1:D:10:GLU:OE1	2.44	0.43
1:D:186:LEU:HB2	1:D:188:LEU:HG	2.01	0.43
1:F:509:ARG:NH2	1:F:884:PRO:HG3	2.34	0.43
1:A:120:MSE:SE	1:A:226:VAL:HG22	2.69	0.43
1:A:473:SER:HA	1:A:515:HIS:O	2.19	0.43
1:A:837:LEU:O	1:A:838:PRO:C	2.57	0.43
1:C:475:ARG:NE	1:C:513:TRP:CE3	2.87	0.43
1:D:558:PRO:HB3	1:D:825:LEU:HD12	2.01	0.43
1:F:125:TRP:CE2	1:F:135:PRO:HG2	2.54	0.43
1:F:307:GLY:N	1:F:308:PRO:CD	2.82	0.42
1:B:238:PHE:HB3	1:B:244:LEU:HG	2.01	0.42
1:C:628:TRP:CZ3	1:C:863:LEU:HD23	2.54	0.42
1:F:615:PRO:O	1:F:618:PHE:HB3	2.19	0.42
1:B:125:TRP:CH2	1:B:135:PRO:HB2	2.54	0.42
1:F:684:GLY:CA	1:F:734:LYS:HB2	2.50	0.42
1:A:620:VAL:HG11	1:A:821:PRO:HG3	2.01	0.42
1:A:880:ALA:O	1:A:881:ASP:HB2	2.20	0.42
1:B:689:GLN:HA	1:B:689:GLN:HE21	1.84	0.42
1:B:663:LEU:HD11	1:B:791:TRP:CE2	2.55	0.42
1:E:529:GLY:O	1:E:533:VAL:HG23	2.20	0.42
1:F:662:LYS:O	1:F:663:LEU:C	2.58	0.42
1:B:398:ARG:HG2	1:B:420:SER:O	2.19	0.42
1:C:568:ALA:O	1:C:572:LEU:HB2	2.20	0.42
1:D:143:THR:HG23	1:D:220:LEU:HB3	2.01	0.42
1:B:40:PRO:HB3	1:B:287:VAL:CG1	2.50	0.42
1:C:758:THR:HG22	1:C:759:GLU:N	2.34	0.42
1:D:120:MSE:HE3	1:D:226:VAL:CG1	2.48	0.42
1:E:867:TYR:HB2	1:E:873:VAL:HG21	2.02	0.42
1:F:145:VAL:O	1:F:192:ALA:HA	2.20	0.42
1:A:683:PHE:CZ	1:A:724:LEU:HD13	2.55	0.42
1:B:294:ASN:HD21	1:B:445:ASN:HB2	1.85	0.42
1:C:834:ASP:O	1:C:836:ALA:N	2.53	0.42
1:F:165:VAL:O	1:F:165:VAL:HG13	2.19	0.42
1:F:203:LEU:HD22	1:F:448:VAL:HG11	2.01	0.42
1:F:600:LEU:HD21	1:F:607:LEU:CD1	2.50	0.42
1:F:705:SER:HB3	1:F:799:VAL:HB	2.01	0.42
1:C:120:MSE:CE	1:C:123:ILE:HD11	2.49	0.42
1:C:143:THR:HG23	1:C:220:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:CYS:SG	1:F:385:MSE:HE1	2.60	0.42
1:D:694:ILE:HG12	1:D:701:LEU:HB2	2.01	0.42
1:E:499:LEU:N	3:E:975:SO4:O4	2.46	0.42
1:C:165:VAL:O	1:C:165:VAL:HG13	2.20	0.42
1:D:141:SER:O	1:D:142:ALA:HB3	2.20	0.42
1:D:491:LEU:HD12	1:D:491:LEU:HA	1.86	0.42
1:D:494:GLU:HG3	1:D:496:ARG:HB3	2.01	0.42
1:F:669:ARG:HG2	1:F:672:ARG:HH12	1.85	0.42
1:A:697:PHE:CD1	1:A:701:LEU:HD12	2.55	0.41
1:B:134:ASP:C	1:B:134:ASP:OD1	2.58	0.41
1:B:157:ARG:O	1:B:158:PRO:C	2.57	0.41
1:C:120:MSE:CE	1:C:266:ALA:HB1	2.50	0.41
1:E:863:LEU:HD22	1:E:873:VAL:CG1	2.49	0.41
1:A:375:THR:HG22	1:A:379:ALA:CA	2.50	0.41
1:B:708:GLY:C	1:B:802:GLN:NE2	2.74	0.41
1:C:186:LEU:N	1:C:186:LEU:HD23	2.36	0.41
1:C:297:GLY:HA2	1:D:188:LEU:O	2.20	0.41
1:F:363:LEU:O	1:F:416:VAL:HA	2.20	0.41
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.84	0.41
1:A:749:VAL:HG12	1:A:749:VAL:O	2.20	0.41
1:B:490:HIS:NE2	1:B:497:ASN:ND2	2.68	0.41
1:C:669:ARG:O	1:C:672:ARG:HB2	2.21	0.41
1:D:522:ASP:O	1:D:523:ARG:C	2.59	0.41
1:D:876:SER:HB2	1:D:877:PRO:HD3	2.02	0.41
1:F:134:ASP:C	1:F:134:ASP:OD1	2.58	0.41
1:C:120:MSE:HA	1:C:120:MSE:HE2	2.02	0.41
1:C:560:GLN:HE21	2:C:950:ACT:CH3	2.33	0.41
1:D:318:LEU:HD23	1:D:449:ILE:HD13	2.01	0.41
1:D:638:VAL:HG21	1:D:652:ALA:HB2	2.02	0.41
1:F:823:PRO:HD3	1:F:849:LEU:O	2.20	0.41
1:B:227:THR:O	1:B:264:GLU:HB2	2.20	0.41
1:D:303:THR:HA	1:D:441:ILE:O	2.21	0.41
1:E:120:MSE:HE3	1:E:226:VAL:HG22	2.01	0.41
1:E:697:PHE:O	1:E:698:ALA:C	2.59	0.41
1:F:113:MSE:HE2	1:F:118:ARG:HG2	2.03	0.41
1:E:522:ASP:O	1:E:523:ARG:C	2.57	0.41
1:F:318:LEU:HD23	1:F:449:ILE:HD13	2.02	0.41
1:B:307:GLY:N	1:B:308:PRO:CD	2.83	0.41
1:C:589:LEU:HD23	1:C:661:ALA:HB1	2.03	0.41
1:D:487:LEU:HA	1:D:487:LEU:HD13	1.82	0.41
1:C:112:ALA:HB2	1:C:165:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:MSE:SE	1:C:226:VAL:HG22	2.71	0.41
1:C:349:LEU:HD13	1:C:365:ILE:HD11	2.03	0.41
1:F:159:ASP:OD1	1:F:159:ASP:N	2.54	0.41
1:A:175:SER:HB3	1:B:196:ASP:OD2	2.20	0.41
1:A:582:ILE:HG23	1:A:597:LEU:HD13	2.03	0.41
1:B:120:MSE:SE	1:B:226:VAL:HG22	2.70	0.41
1:C:134:ASP:OD2	1:C:511:SER:HA	2.21	0.41
1:C:560:GLN:NE2	2:C:950:ACT:C	2.84	0.41
1:E:639:VAL:CG2	1:E:808:LEU:HD11	2.50	0.41
1:B:628:TRP:CZ3	1:B:863:LEU:HD23	2.56	0.41
1:C:671:LEU:HD13	1:C:795:LEU:HD11	2.02	0.41
1:D:125:TRP:CE2	1:D:135:PRO:HG2	2.55	0.41
1:F:685:LEU:HD22	1:F:689:GLN:HB3	2.02	0.41
1:F:744:SER:HB2	1:F:745:HIS:CD2	2.56	0.41
1:F:856:LEU:HA	1:F:856:LEU:HD23	1.92	0.41
1:A:590:ALA:N	1:A:591:PRO:HD2	2.36	0.41
1:B:511:SER:HB2	1:B:513:TRP:CE2	2.56	0.41
1:D:342:ASP:HB2	1:D:343:PRO:HD3	2.03	0.41
1:E:376:GLN:O	1:E:377:ALA:C	2.59	0.41
1:E:514:GLU:HB2	5:E:1012:HOH:O	2.21	0.41
1:F:46:MSE:HE2	1:F:269:LEU:HD11	2.02	0.41
1:A:294:ASN:HD21	1:A:445:ASN:HB2	1.85	0.40
1:C:291:SER:HB3	1:C:448:VAL:HG23	2.02	0.40
1:A:541:ARG:NH1	1:A:858:ASP:OD1	2.54	0.40
1:B:899:LEU:HA	1:B:900:PRO:HD3	1.87	0.40
1:D:819:VAL:HG12	1:D:819:VAL:O	2.21	0.40
1:E:206:LEU:HD23	1:E:206:LEU:C	2.42	0.40
1:C:688:GLU:O	1:C:692:GLU:CG	2.66	0.40
1:C:806:ARG:HB3	1:C:806:ARG:CZ	2.51	0.40
1:D:850:ARG:CG	1:D:851:ARG:N	2.85	0.40
1:A:122:GLU:O	1:A:126:GLU:HG3	2.21	0.40
1:A:696:ARG:HB3	5:A:988:HOH:O	2.20	0.40
1:B:475:ARG:HG2	1:B:890:TYR:OH	2.21	0.40
1:C:16:LEU:O	1:C:17:LYS:C	2.58	0.40
1:D:494:GLU:HG3	1:D:496:ARG:CB	2.52	0.40
1:A:838:PRO:HB2	1:A:841:ALA:HB3	2.04	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.97	0.40
1:B:491:LEU:HA	1:B:491:LEU:HD12	1.90	0.40
1:C:93:ALA:N	5:C:981:HOH:O	2.55	0.40
1:D:494:GLU:CD	1:D:495:PRO:HD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	876/917 (96%)	823 (94%)	43 (5%)	10 (1%)	14	26
1	B	876/917 (96%)	813 (93%)	55 (6%)	8 (1%)	17	32
1	C	876/917 (96%)	796 (91%)	69 (8%)	11 (1%)	12	21
1	D	876/917 (96%)	808 (92%)	58 (7%)	10 (1%)	14	26
1	E	871/917 (95%)	795 (91%)	65 (8%)	11 (1%)	12	21
1	F	870/917 (95%)	795 (91%)	61 (7%)	14 (2%)	9	17
All	All	5245/5502 (95%)	4830 (92%)	351 (7%)	64 (1%)	13	24

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ASP
1	A	567	MSE
1	B	403	ASP
1	B	698	ALA
1	C	687	THR
1	D	403	ASP
1	D	567	MSE
1	D	843	ALA
1	E	175	SER
1	E	403	ASP
1	E	523	ARG
1	E	698	ALA
1	E	843	ALA
1	F	360	ASP
1	F	416	VAL
1	F	567	MSE
1	A	698	ALA
1	B	240	SER
1	C	497	ASN
1	C	698	ALA

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Mol	Chain	Res	Type
1	C	758	THR
1	C	769	ASP
1	C	855	GLY
1	D	698	ALA
1	E	360	ASP
1	E	567	MSE
1	F	403	ASP
1	F	769	ASP
1	F	840	ASP
1	A	93	ALA
1	A	202	GLY
1	A	360	ASP
1	A	732	ALA
1	B	567	MSE
1	B	855	GLY
1	C	429	GLU
1	C	642	SER
1	C	835	SER
1	D	216	ASP
1	D	842	GLY
1	E	643	GLN
1	F	642	SER
1	F	855	GLY
1	A	335	GLY
1	B	800	ARG
1	D	242	GLY
1	A	416	VAL
1	A	900	PRO
1	B	838	PRO
1	C	416	VAL
1	C	493	ARG
1	D	416	VAL
1	D	496	ARG
1	E	376	GLN
1	E	416	VAL
1	F	24	ASP
1	F	826	THR
1	F	900	PRO
1	B	416	VAL
1	F	22	GLU
1	F	758	THR
1	E	900	PRO

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Mol	Chain	Res	Type
1	D	819	VAL
1	F	577	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	647/668 (97%)	558 (86%)	89 (14%)	3 4
1	B	650/668 (97%)	581 (89%)	69 (11%)	6 11
1	C	647/668 (97%)	571 (88%)	76 (12%)	5 8
1	D	652/668 (98%)	572 (88%)	80 (12%)	4 7
1	E	643/668 (96%)	579 (90%)	64 (10%)	7 13
1	F	638/668 (96%)	561 (88%)	77 (12%)	5 8
All	All	3877/4008 (97%)	3422 (88%)	455 (12%)	5 8

All (455) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LYS
1	A	18	ARG
1	A	23	LEU
1	A	29	ARG
1	A	31	ARG
1	A	36	ARG
1	A	44	VAL
1	A	46	MSE
1	A	49	ARG
1	A	92	LEU
1	A	165	VAL
1	A	166	LEU
1	A	171	THR
1	A	175	SER
1	A	179	SER

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Mol	Chain	Res	Type
1	A	186	LEU
1	A	226	VAL
1	A	249	ARG
1	A	258	ASP
1	A	268	VAL
1	A	289	ARG
1	A	294	ASN
1	A	306	SER
1	A	320	ASN
1	A	357	ARG
1	A	360	ASP
1	A	363	LEU
1	A	368	VAL
1	A	374	HIS
1	A	375	THR
1	A	419	VAL
1	A	430	ARG
1	A	433	ARG
1	A	437	SER
1	A	438	SER
1	A	441	ILE
1	A	457	ASP
1	A	471	VAL
1	A	475	ARG
1	A	487	LEU
1	A	494	GLU
1	A	509	ARG
1	A	511	SER
1	A	523	ARG
1	A	540	ASP
1	A	541	ARG
1	A	544	THR
1	A	548	ARG
1	A	551	ARG
1	A	563	GLN
1	A	572	LEU
1	A	583	ARG
1	A	597	LEU
1	A	600	LEU
1	A	607	LEU
1	A	610	VAL
1	A	617	LEU

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Mol	Chain	Res	Type
1	A	663	LEU
1	A	682	SER
1	A	685	LEU
1	A	689	GLN
1	A	696	ARG
1	A	706	VAL
1	A	712	VAL
1	A	724	LEU
1	A	734	LYS
1	A	736	ARG
1	A	740	VAL
1	A	741	ASP
1	A	750	GLU
1	A	763	ILE
1	A	769	ASP
1	A	772	LEU
1	A	775	THR
1	A	794	ASN
1	A	795	LEU
1	A	800	ARG
1	A	814	ASP
1	A	818	GLU
1	A	826	THR
1	A	834	ASP
1	A	835	SER
1	A	856	LEU
1	A	872	GLU
1	A	876	SER
1	A	885	VAL
1	A	889	VAL
1	A	899	LEU
1	B	12	LEU
1	B	14	ARG
1	B	15	TYR
1	B	18	ARG
1	B	29	ARG
1	B	151	THR
1	B	165	VAL
1	B	179	SER
1	B	186	LEU
1	B	206	LEU
1	B	212	SER

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Mol	Chain	Res	Type
1	B	226	VAL
1	B	241	GLN
1	B	268	VAL
1	B	289	ARG
1	B	294	ASN
1	B	300	ASN
1	B	306	SER
1	B	313	VAL
1	B	324	ARG
1	B	329	ASP
1	B	340	LEU
1	B	360	ASP
1	B	368	VAL
1	B	398	ARG
1	B	419	VAL
1	B	430	ARG
1	B	433	ARG
1	B	441	ILE
1	B	473	SER
1	B	475	ARG
1	B	477	GLU
1	B	487	LEU
1	B	491	LEU
1	B	511	SER
1	B	541	ARG
1	B	544	THR
1	B	548	ARG
1	B	563	GLN
1	B	593	VAL
1	B	597	LEU
1	B	600	LEU
1	B	607	LEU
1	B	608	ASP
1	B	617	LEU
1	B	630	SER
1	B	658	GLU
1	B	663	LEU
1	B	685	LEU
1	B	689	GLN
1	B	712	VAL
1	B	724	LEU
1	B	734	LYS

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Mol	Chain	Res	Type
1	B	740	VAL
1	B	741	ASP
1	B	746	SER
1	B	750	GLU
1	B	753	ARG
1	B	772	LEU
1	B	794	ASN
1	B	795	LEU
1	B	800	ARG
1	B	803	ASP
1	B	818	GLU
1	B	872	GLU
1	B	885	VAL
1	B	886	GLU
1	B	899	LEU
1	B	900	PRO
1	C	10	GLU
1	C	18	ARG
1	C	20	VAL
1	C	29	ARG
1	C	31	ARG
1	C	41	ILE
1	C	49	ARG
1	C	92	LEU
1	C	97	ASP
1	C	159	ASP
1	C	164	GLU
1	C	165	VAL
1	C	171	THR
1	C	200	SER
1	C	226	VAL
1	C	231	SER
1	C	240	SER
1	C	268	VAL
1	C	289	ARG
1	C	294	ASN
1	C	327	ASP
1	C	340	LEU
1	C	357	ARG
1	C	358	ASP
1	C	360	ASP
1	C	368	VAL

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Mol	Chain	Res	Type
1	C	375	THR
1	C	419	VAL
1	C	424	SER
1	C	430	ARG
1	C	433	ARG
1	C	437	SER
1	C	441	ILE
1	C	471	VAL
1	C	475	ARG
1	C	511	SER
1	C	525	GLU
1	C	541	ARG
1	C	544	THR
1	C	550	ARG
1	C	551	ARG
1	C	563	GLN
1	C	570	ASP
1	C	572	LEU
1	C	583	ARG
1	C	597	LEU
1	C	600	LEU
1	C	607	LEU
1	C	617	LEU
1	C	627	LEU
1	C	658	GLU
1	C	663	LEU
1	C	685	LEU
1	C	687	THR
1	C	689	GLN
1	C	696	ARG
1	C	706	VAL
1	C	712	VAL
1	C	724	LEU
1	C	734	LYS
1	C	736	ARG
1	C	740	VAL
1	C	750	GLU
1	C	759	GLU
1	C	769	ASP
1	C	772	LEU
1	C	775	THR
1	C	795	LEU

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Mol	Chain	Res	Type
1	C	800	ARG
1	C	803	ASP
1	C	826	THR
1	C	844	CYS
1	C	872	GLU
1	C	889	VAL
1	C	896	ARG
1	C	899	LEU
1	D	8	THR
1	D	12	LEU
1	D	16	LEU
1	D	17	LYS
1	D	23	LEU
1	D	30	LEU
1	D	31	ARG
1	D	44	VAL
1	D	46	MSE
1	D	49	ARG
1	D	97	ASP
1	D	164	GLU
1	D	165	VAL
1	D	166	LEU
1	D	171	THR
1	D	175	SER
1	D	226	VAL
1	D	247	ASP
1	D	268	VAL
1	D	289	ARG
1	D	294	ASN
1	D	306	SER
1	D	324	ARG
1	D	340	LEU
1	D	356	GLU
1	D	361	ASP
1	D	365	ILE
1	D	368	VAL
1	D	398	ARG
1	D	419	VAL
1	D	424	SER
1	D	430	ARG
1	D	433	ARG
1	D	441	ILE

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Mol	Chain	Res	Type
1	D	468	VAL
1	D	471	VAL
1	D	475	ARG
1	D	491	LEU
1	D	494	GLU
1	D	541	ARG
1	D	548	ARG
1	D	549	THR
1	D	550	ARG
1	D	551	ARG
1	D	563	GLN
1	D	572	LEU
1	D	593	VAL
1	D	597	LEU
1	D	600	LEU
1	D	607	LEU
1	D	608	ASP
1	D	617	LEU
1	D	627	LEU
1	D	639	VAL
1	D	663	LEU
1	D	669	ARG
1	D	682	SER
1	D	685	LEU
1	D	689	GLN
1	D	696	ARG
1	D	706	VAL
1	D	712	VAL
1	D	724	LEU
1	D	734	LYS
1	D	736	ARG
1	D	740	VAL
1	D	750	GLU
1	D	769	ASP
1	D	772	LEU
1	D	795	LEU
1	D	800	ARG
1	D	810	GLU
1	D	835	SER
1	D	840	ASP
1	D	844	CYS
1	D	858	ASP

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Mol	Chain	Res	Type
1	D	869	GLN
1	D	872	GLU
1	D	883	ARG
1	D	889	VAL
1	E	18	ARG
1	E	23	LEU
1	E	30	LEU
1	E	44	VAL
1	E	46	MSE
1	E	49	ARG
1	E	85	ASP
1	E	92	LEU
1	E	159	ASP
1	E	165	VAL
1	E	166	LEU
1	E	171	THR
1	E	200	SER
1	E	212	SER
1	E	226	VAL
1	E	240	SER
1	E	251	LYS
1	E	273	ARG
1	E	289	ARG
1	E	294	ASN
1	E	306	SER
1	E	324	ARG
1	E	340	LEU
1	E	352	THR
1	E	360	ASP
1	E	368	VAL
1	E	423	ARG
1	E	430	ARG
1	E	433	ARG
1	E	441	ILE
1	E	471	VAL
1	E	491	LEU
1	E	525	GLU
1	E	541	ARG
1	E	542	THR
1	E	548	ARG
1	E	550	ARG
1	E	563	GLN

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Mol	Chain	Res	Type
1	E	572	LEU
1	E	593	VAL
1	E	597	LEU
1	E	600	LEU
1	E	617	LEU
1	E	627	LEU
1	E	639	VAL
1	E	663	LEU
1	E	685	LEU
1	E	692	GLU
1	E	696	ARG
1	E	706	VAL
1	E	712	VAL
1	E	734	LYS
1	E	741	ASP
1	E	750	GLU
1	E	753	ARG
1	E	769	ASP
1	E	772	LEU
1	E	795	LEU
1	E	800	ARG
1	E	844	CYS
1	E	872	GLU
1	E	876	SER
1	E	885	VAL
1	E	889	VAL
1	F	29	ARG
1	F	49	ARG
1	F	59	SER
1	F	92	LEU
1	F	151	THR
1	F	159	ASP
1	F	165	VAL
1	F	166	LEU
1	F	173	THR
1	F	176	SER
1	F	197	THR
1	F	226	VAL
1	F	231	SER
1	F	247	ASP
1	F	268	VAL
1	F	289	ARG

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Mol	Chain	Res	Type
1	F	294	ASN
1	F	306	SER
1	F	340	LEU
1	F	357	ARG
1	F	361	ASP
1	F	363	LEU
1	F	365	ILE
1	F	368	VAL
1	F	374	HIS
1	F	419	VAL
1	F	424	SER
1	F	430	ARG
1	F	433	ARG
1	F	437	SER
1	F	441	ILE
1	F	487	LEU
1	F	491	LEU
1	F	496	ARG
1	F	500	ARG
1	F	511	SER
1	F	535	ASP
1	F	540	ASP
1	F	541	ARG
1	F	544	THR
1	F	550	ARG
1	F	551	ARG
1	F	563	GLN
1	F	572	LEU
1	F	583	ARG
1	F	597	LEU
1	F	598	THR
1	F	600	LEU
1	F	607	LEU
1	F	609	ARG
1	F	617	LEU
1	F	627	LEU
1	F	663	LEU
1	F	669	ARG
1	F	685	LEU
1	F	688	GLU
1	F	696	ARG
1	F	706	VAL

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Mol	Chain	Res	Type
1	F	718	SER
1	F	724	LEU
1	F	734	LYS
1	F	736	ARG
1	F	740	VAL
1	F	769	ASP
1	F	772	LEU
1	F	780	PRO
1	F	795	LEU
1	F	800	ARG
1	F	803	ASP
1	F	814	ASP
1	F	818	GLU
1	F	826	THR
1	F	850	ARG
1	F	865	GLU
1	F	876	SER
1	F	889	VAL
1	F	899	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	320	ASN
1	A	445	ASN
1	A	689	GLN
1	A	748	GLN
1	A	802	GLN
1	B	241	GLN
1	B	294	ASN
1	B	300	ASN
1	B	445	ASN
1	B	483	GLN
1	B	497	ASN
1	B	560	GLN
1	B	689	GLN
1	B	802	GLN
1	B	860	HIS
1	C	294	ASN
1	C	320	ASN
1	C	334	HIS

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Mol	Chain	Res	Type
1	C	478	GLN
1	C	483	GLN
1	C	560	GLN
1	C	643	GLN
1	D	294	ASN
1	D	376	GLN
1	D	445	ASN
1	D	497	ASN
1	D	560	GLN
1	D	689	GLN
1	D	802	GLN
1	D	807	GLN
1	E	294	ASN
1	E	334	HIS
1	E	490	HIS
1	E	497	ASN
1	F	294	ASN
1	F	334	HIS
1	F	445	ASN
1	F	560	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	F	950	-	1,3,3	1.72	0	0,3,3	0.00	-
2	ACT	A	950	-	1,3,3	1.06	0	0,3,3	0.00	-
2	ACT	C	950	-	1,3,3	1.32	0	0,3,3	0.00	-
2	ACT	B	950	-	1,3,3	1.27	0	0,3,3	0.00	-
2	ACT	E	950	-	1,3,3	0.57	0	0,3,3	0.00	-
3	SO4	E	975	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	B	975	-	4,4,4	0.06	0	6,6,6	0.26	0
3	SO4	A	975	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	C	975	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	F	975	-	4,4,4	0.16	0	6,6,6	0.40	0
2	ACT	D	950	-	1,3,3	1.86	0	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	950	ACT	1	0
2	C	950	ACT	4	0
2	B	950	ACT	2	0
2	E	950	ACT	1	0
3	E	975	SO4	1	0
3	B	975	SO4	1	0
2	D	950	ACT	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	867/917 (94%)	0.54	58 (6%) 17 20	34, 67, 80, 94	0
1	B	867/917 (94%)	0.66	71 (8%) 11 13	46, 67, 80, 93	0
1	C	867/917 (94%)	0.72	85 (9%) 7 7	47, 67, 80, 93	0
1	D	868/917 (94%)	0.70	87 (10%) 7 7	48, 67, 80, 93	0
1	E	862/917 (94%)	0.67	76 (8%) 10 10	48, 67, 81, 93	0
1	F	859/917 (93%)	0.66	80 (9%) 8 9	48, 67, 80, 93	0
All	All	5190/5502 (94%)	0.66	457 (8%) 10 10	34, 67, 80, 94	0

All (457) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	8.0
1	C	496	ARG	7.1
1	B	840	ASP	6.9
1	C	551	ARG	6.8
1	D	551	ARG	6.4
1	B	360	ASP	6.2
1	F	24	ASP	6.0
1	E	551	ARG	5.9
1	E	253	PHE	5.9
1	E	732	ALA	5.6
1	E	497	ASN	5.6
1	C	359	PRO	5.5
1	B	560	GLN	5.3
1	F	22	GLU	5.3
1	C	760	LEU	5.1
1	E	883	ARG	5.1
1	C	15	TYR	5.1
1	D	732	ALA	5.0
1	F	551	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	241	GLN	4.9
1	E	496	ARG	4.9
1	F	837	LEU	4.6
1	F	602	SER	4.6
1	D	601	LEU	4.6
1	D	560	GLN	4.6
1	C	497	ASN	4.6
1	E	466	GLY	4.5
1	D	416	VAL	4.5
1	A	163	ASP	4.5
1	A	607	LEU	4.5
1	E	736	ARG	4.5
1	C	756	LEU	4.4
1	C	694	ILE	4.4
1	E	22	GLU	4.3
1	E	537	ARG	4.3
1	F	21	THR	4.3
1	D	728	CYS	4.3
1	C	607	LEU	4.3
1	D	720	PRO	4.3
1	D	681	ALA	4.2
1	E	880	ALA	4.2
1	C	12	LEU	4.2
1	C	769	ASP	4.1
1	B	355	ALA	4.1
1	A	551	ARG	4.1
1	E	536	GLY	4.1
1	E	733	HIS	4.1
1	B	551	ARG	4.1
1	E	715	ALA	4.1
1	F	839	ALA	4.1
1	E	33	VAL	4.0
1	D	359	PRO	4.0
1	E	837	LEU	4.0
1	F	683	PHE	4.0
1	F	595	TRP	3.9
1	F	608	ASP	3.9
1	D	408	GLN	3.9
1	D	716	GLY	3.9
1	E	729	GLU	3.9
1	D	679	GLY	3.9
1	A	360	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	18	ARG	3.8
1	C	801	PHE	3.8
1	A	769	ASP	3.8
1	A	595	TRP	3.8
1	E	726	ALA	3.8
1	F	456	ALA	3.8
1	B	736	ARG	3.8
1	B	356	GLU	3.8
1	D	600	LEU	3.7
1	B	11	LYS	3.7
1	C	53	ASP	3.7
1	F	836	ALA	3.7
1	E	728	CYS	3.7
1	E	881	ASP	3.7
1	D	495	PRO	3.7
1	C	595	TRP	3.7
1	D	379	ALA	3.7
1	E	356	GLU	3.7
1	C	552	GLY	3.7
1	C	84	PRO	3.6
1	D	900	PRO	3.6
1	F	414	GLY	3.6
1	D	742	TYR	3.5
1	F	360	ASP	3.5
1	A	456	ALA	3.5
1	F	496	ARG	3.5
1	C	176	SER	3.5
1	A	457	ASP	3.5
1	F	26	VAL	3.5
1	B	841	ALA	3.5
1	A	742	TYR	3.4
1	C	566	GLY	3.4
1	C	573	ARG	3.4
1	D	456	ALA	3.4
1	D	537	ARG	3.4
1	D	430	ARG	3.4
1	F	637	ALA	3.4
1	E	412	ASP	3.4
1	D	608	ASP	3.3
1	F	175	SER	3.3
1	C	241	GLN	3.3
1	E	534	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	837	LEU	3.3
1	A	840	ASP	3.3
1	C	741	ASP	3.3
1	E	470	LEU	3.3
1	E	683	PHE	3.2
1	B	340	LEU	3.2
1	C	147	THR	3.2
1	F	804	ALA	3.2
1	D	14	ARG	3.2
1	D	159	ASP	3.2
1	C	773	TYR	3.2
1	F	356	GLU	3.2
1	A	454	PRO	3.2
1	D	84	PRO	3.2
1	E	17	LYS	3.2
1	D	493	ARG	3.2
1	C	810	GLU	3.1
1	C	177	VAL	3.1
1	D	683	PHE	3.1
1	A	169	VAL	3.1
1	E	687	THR	3.1
1	B	719	GLY	3.1
1	E	360	ASP	3.1
1	F	81	GLU	3.1
1	F	713	VAL	3.1
1	F	799	VAL	3.1
1	A	773	TYR	3.1
1	B	839	ALA	3.1
1	B	537	ARG	3.1
1	A	815	ALA	3.1
1	E	420	SER	3.1
1	F	690	ALA	3.1
1	F	636	ALA	3.0
1	C	228	VAL	3.0
1	E	602	SER	3.0
1	B	176	SER	3.0
1	E	64	VAL	3.0
1	F	833	LEU	3.0
1	F	816	PHE	3.0
1	D	147	THR	3.0
1	C	226	VAL	3.0
1	C	360	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	743	ALA	3.0
1	F	800	ARG	3.0
1	D	671	LEU	3.0
1	E	518	VAL	3.0
1	C	415	ALA	3.0
1	C	737	ARG	3.0
1	C	495	PRO	3.0
1	B	225	GLY	3.0
1	B	14	ARG	3.0
1	C	242	GLY	2.9
1	C	86	ALA	2.9
1	C	839	ALA	2.9
1	E	495	PRO	2.9
1	B	419	VAL	2.9
1	E	30	LEU	2.9
1	D	64	VAL	2.9
1	B	681	ALA	2.9
1	F	495	PRO	2.9
1	C	840	ASP	2.9
1	F	583	ARG	2.9
1	F	25	SER	2.9
1	D	357	ARG	2.9
1	F	689	GLN	2.9
1	E	31	ARG	2.9
1	D	356	GLU	2.8
1	C	837	LEU	2.8
1	D	470	LEU	2.8
1	C	493	ARG	2.8
1	B	198	ALA	2.8
1	B	415	ALA	2.8
1	C	547	ALA	2.8
1	F	359	PRO	2.8
1	B	353	TYR	2.8
1	F	357	ARG	2.8
1	B	583	ARG	2.8
1	D	538	ILE	2.8
1	A	552	GLY	2.8
1	B	242	GLY	2.8
1	B	359	PRO	2.8
1	A	14	ARG	2.8
1	B	201	SER	2.8
1	F	242	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	430	ARG	2.8
1	F	248	GLY	2.8
1	A	84	PRO	2.8
1	D	838	PRO	2.8
1	D	410	GLU	2.8
1	E	21	THR	2.8
1	D	76	ALA	2.7
1	C	148	GLY	2.7
1	A	147	THR	2.7
1	D	743	ALA	2.7
1	D	731	GLU	2.7
1	B	226	VAL	2.7
1	B	768	ALA	2.7
1	E	252	PRO	2.7
1	F	619	ALA	2.7
1	A	608	ASP	2.7
1	B	138	LEU	2.7
1	D	497	ASN	2.7
1	A	194	THR	2.7
1	C	194	THR	2.7
1	D	166	LEU	2.7
1	F	358	ASP	2.7
1	F	415	ALA	2.7
1	D	500	ARG	2.7
1	F	194	THR	2.7
1	B	405	PRO	2.7
1	E	24	ASP	2.7
1	E	419	VAL	2.7
1	C	854	GLY	2.7
1	E	573	ARG	2.7
1	E	467	PRO	2.7
1	C	739	PRO	2.6
1	F	148	GLY	2.6
1	D	62	GLU	2.6
1	A	771	ALA	2.6
1	D	730	ALA	2.6
1	F	732	ALA	2.6
1	C	671	LEU	2.6
1	D	724	LEU	2.6
1	A	811	ALA	2.6
1	A	145	VAL	2.6
1	D	225	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	604	ALA	2.6
1	F	840	ASP	2.6
1	A	810	GLU	2.6
1	C	10	GLU	2.6
1	C	678	GLY	2.6
1	C	23	LEU	2.6
1	C	540	ASP	2.6
1	D	340	LEU	2.6
1	A	455	GLU	2.6
1	E	339	ARG	2.6
1	F	838	PRO	2.6
1	A	839	ALA	2.6
1	D	415	ALA	2.6
1	F	691	ALA	2.6
1	C	749	VAL	2.6
1	D	602	SER	2.6
1	B	880	ALA	2.5
1	C	841	ALA	2.5
1	C	792	TYR	2.5
1	C	169	VAL	2.5
1	E	840	ASP	2.5
1	F	167	GLY	2.5
1	C	776	THR	2.5
1	A	12	LEU	2.5
1	A	835	SER	2.5
1	D	590	ALA	2.5
1	E	488	ALA	2.5
1	D	851	ARG	2.5
1	F	764	SER	2.5
1	A	549	THR	2.5
1	B	505	THR	2.5
1	F	747	PRO	2.5
1	B	148	GLY	2.5
1	E	430	ARG	2.5
1	A	600	LEU	2.5
1	A	816	PHE	2.5
1	D	360	ASP	2.5
1	F	540	ASP	2.5
1	A	266	ALA	2.5
1	C	14	ARG	2.5
1	D	595	TRP	2.5
1	E	589	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	62	GLU	2.5
1	F	692	GLU	2.5
1	F	147	THR	2.5
1	B	395	GLU	2.5
1	A	33	VAL	2.5
1	B	790	TYR	2.5
1	C	742	TYR	2.5
1	C	767	SER	2.5
1	E	254	SER	2.5
1	C	541	ARG	2.5
1	F	611	ASP	2.5
1	B	147	THR	2.5
1	C	18	ARG	2.5
1	D	719	GLY	2.4
1	A	604	ALA	2.4
1	C	174	ALA	2.4
1	D	880	ALA	2.4
1	E	147	THR	2.4
1	C	470	LEU	2.4
1	E	875	TRP	2.4
1	E	148	GLY	2.4
1	F	739	PRO	2.4
1	D	836	ALA	2.4
1	B	199	CYS	2.4
1	B	377	ALA	2.4
1	C	355	ALA	2.4
1	E	517	ALA	2.4
1	B	813	PHE	2.4
1	D	840	ASP	2.4
1	D	867	TYR	2.4
1	F	728	CYS	2.4
1	A	800	ARG	2.4
1	F	605	ARG	2.4
1	A	340	LEU	2.4
1	E	607	LEU	2.4
1	F	599	ASP	2.4
1	D	148	GLY	2.4
1	A	151	THR	2.4
1	C	856	LEU	2.4
1	D	839	ALA	2.4
1	F	756	LEU	2.4
1	F	570	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	224	GLY	2.4
1	E	716	GLY	2.4
1	B	838	PRO	2.4
1	A	378	ALA	2.4
1	B	714	VAL	2.4
1	D	816	PHE	2.4
1	F	792	TYR	2.3
1	C	772	LEU	2.3
1	D	198	ALA	2.3
1	F	872	GLU	2.3
1	A	689	GLN	2.3
1	E	25	SER	2.3
1	E	499	LEU	2.3
1	A	872	GLU	2.3
1	C	855	GLY	2.3
1	F	179	SER	2.3
1	C	612	VAL	2.3
1	C	821	PRO	2.3
1	B	655	LEU	2.3
1	D	744	SER	2.3
1	D	792	TYR	2.3
1	E	867	TYR	2.3
1	C	95	ALA	2.3
1	C	145	VAL	2.3
1	F	457	ASP	2.3
1	B	812	GLY	2.3
1	C	166	LEU	2.3
1	C	225	GLY	2.3
1	E	719	GLY	2.3
1	A	556	VAL	2.3
1	E	608	ASP	2.3
1	E	882	ALA	2.3
1	D	22	GLU	2.3
1	C	85	ASP	2.3
1	F	773	TYR	2.3
1	B	10	GLU	2.3
1	E	455	GLU	2.3
1	A	801	PHE	2.3
1	A	379	ALA	2.3
1	E	507	ALA	2.3
1	D	583	ARG	2.3
1	E	801	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	639	VAL	2.3
1	F	552	GLY	2.2
1	B	347	HIS	2.2
1	E	411	TRP	2.2
1	F	407	PRO	2.2
1	C	560	GLN	2.2
1	A	692	GLU	2.2
1	A	225	GLY	2.2
1	A	265	GLY	2.2
1	E	350	LEU	2.2
1	C	192	ALA	2.2
1	D	365	ILE	2.2
1	F	177	VAL	2.2
1	B	48	CYS	2.2
1	A	580	ASP	2.2
1	B	444	THR	2.2
1	B	826	THR	2.2
1	D	549	THR	2.2
1	A	326	GLY	2.2
1	C	164	GLU	2.2
1	C	762	GLY	2.2
1	B	639	VAL	2.2
1	F	609	ARG	2.2
1	A	197	THR	2.2
1	A	881	ASP	2.2
1	F	726	ALA	2.2
1	B	504	PHE	2.2
1	B	468	VAL	2.2
1	D	670	VAL	2.2
1	F	901	ILE	2.2
1	E	655	LEU	2.2
1	D	717	GLU	2.2
1	C	197	THR	2.2
1	B	850	ARG	2.2
1	D	737	ARG	2.2
1	B	350	LEU	2.2
1	E	164	GLU	2.2
1	E	530	LEU	2.2
1	F	719	GLY	2.2
1	D	353	TYR	2.1
1	D	714	VAL	2.1
1	F	763	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	503	GLY	2.1
1	B	500	ARG	2.1
1	A	34	GLU	2.1
1	B	260	PHE	2.1
1	A	228	VAL	2.1
1	B	53	ASP	2.1
1	D	163	ASP	2.1
1	D	457	ASP	2.1
1	B	392	ARG	2.1
1	B	587	ARG	2.1
1	C	73	GLU	2.1
1	E	484	ALA	2.1
1	F	562	ALA	2.1
1	B	253	PHE	2.1
1	A	500	ARG	2.1
1	C	149	VAL	2.1
1	B	256	ALA	2.1
1	B	324	ARG	2.1
1	B	710	ARG	2.1
1	A	671	LEU	2.1
1	B	733	HIS	2.1
1	D	799	VAL	2.1
1	D	897	TYR	2.1
1	C	660	ALA	2.1
1	E	421	GLN	2.1
1	C	788	THR	2.1
1	A	324	ARG	2.1
1	D	324	ARG	2.1
1	C	265	GLY	2.1
1	B	588	ALA	2.1
1	C	246	ALA	2.1
1	C	815	ALA	2.1
1	C	857	ALA	2.1
1	D	361	ASP	2.1
1	D	535	ASP	2.1
1	D	817	VAL	2.1
1	E	199	CYS	2.1
1	C	266	ALA	2.1
1	F	525	GLU	2.1
1	B	769	ASP	2.1
1	F	150	GLY	2.1
1	E	724	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	565	GLN	2.0
1	B	742	TYR	2.0
1	C	324	ARG	2.0
1	E	658	GLU	2.0
1	A	375	THR	2.0
1	F	560	GLN	2.0
1	D	413	LEU	2.0
1	D	715	ALA	2.0
1	D	111	LEU	2.0
1	F	455	GLU	2.0
1	A	192	ALA	2.0
1	B	867	TYR	2.0
1	D	380	GLY	2.0
1	E	366	GLY	2.0
1	F	427	ALA	2.0
1	E	689	GLN	2.0
1	B	60	PHE	2.0
1	B	36	ARG	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. 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	SO4	C	975	5/5	0.75	0.42	84,84,85,86	5
3	SO4	E	975	5/5	0.76	0.30	101,101,102,102	5
4	CL	F	976	1/1	0.76	0.25	76,76,76,76	0
4	CL	E	976	1/1	0.81	0.17	70,70,70,70	0
3	SO4	B	975	5/5	0.84	0.36	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	C	976	1/1	0.85	0.23	82,82,82,82	0
4	CL	B	976	1/1	0.88	0.13	57,57,57,57	0
2	ACT	F	950	4/4	0.91	0.18	44,44,45,45	0
3	SO4	A	975	5/5	0.91	0.30	87,87,88,88	0
2	ACT	D	950	4/4	0.92	0.17	61,61,61,62	0
3	SO4	F	975	5/5	0.94	0.35	82,82,83,83	0
2	ACT	B	950	4/4	0.94	0.12	50,50,50,50	0
2	ACT	A	950	4/4	0.94	0.10	51,51,51,51	0
4	CL	D	951	1/1	0.95	0.13	90,90,90,90	0
2	ACT	E	950	4/4	0.96	0.11	47,48,48,48	0
2	ACT	C	950	4/4	0.96	0.15	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.