



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:03 PM UTC

PDB ID : 2HG4 / pdb_00002hg4
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

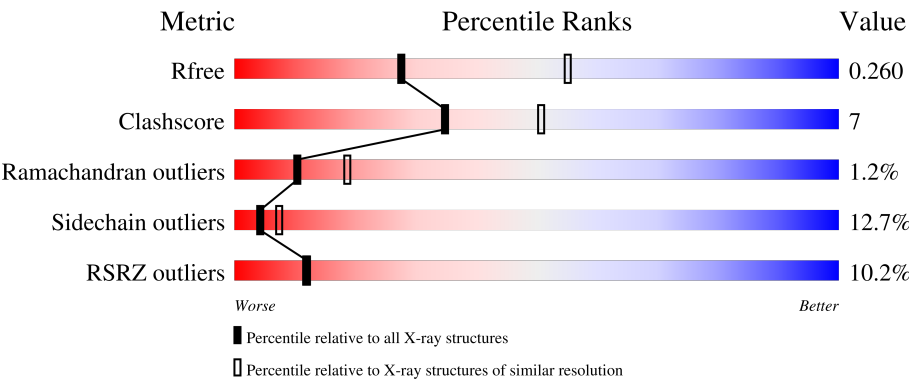
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	917	4% 74% 18% ...
1	B	917	7% 74% 20% ..
1	C	917	9% 75% 18% ..
1	D	917	20% 75% 18% ..
1	E	917	9% 78% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	917	

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	-

2 Entry composition [i](#)

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
C	120	MSE	MET	modified residue	UNP Q5UNP4
C	193	MSE	MET	modified residue	UNP Q5UNP4
C	210	MSE	MET	modified residue	UNP Q5UNP4
C	229	MSE	MET	modified residue	UNP Q5UNP4
C	385	MSE	MET	modified residue	UNP Q5UNP4
C	396	MSE	MET	modified residue	UNP Q5UNP4
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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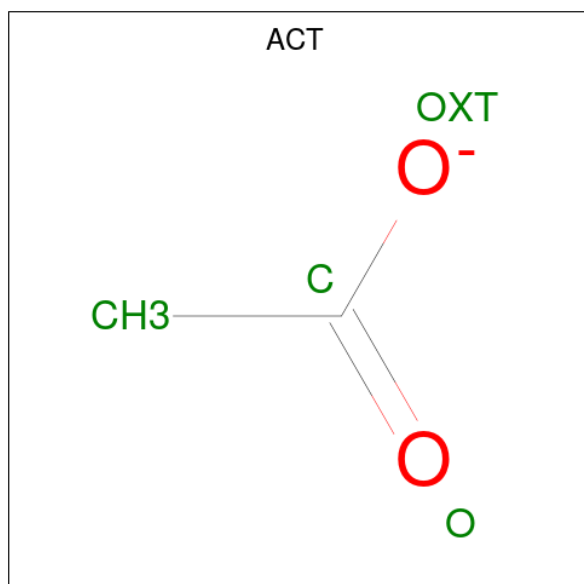
Chain	Residue	Modelled	Actual	Comment	Reference
C	732	ALA	GLY	conflict	UNP Q5UNP4
C	733	HIS	ILE	conflict	UNP Q5UNP4
C	734	LYS	THR	conflict	UNP Q5UNP4
C	786	MSE	MET	modified residue	UNP Q5UNP4
D	1	MSE	MET	modified residue	UNP Q5UNP4
D	7	MSE	MET	modified residue	UNP Q5UNP4
D	46	MSE	MET	modified residue	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
D	210	MSE	MET	modified residue	UNP Q5UNP4
D	229	MSE	MET	modified residue	UNP Q5UNP4
D	385	MSE	MET	modified residue	UNP Q5UNP4
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
D	732	ALA	GLY	conflict	UNP Q5UNP4
D	733	HIS	ILE	conflict	UNP Q5UNP4
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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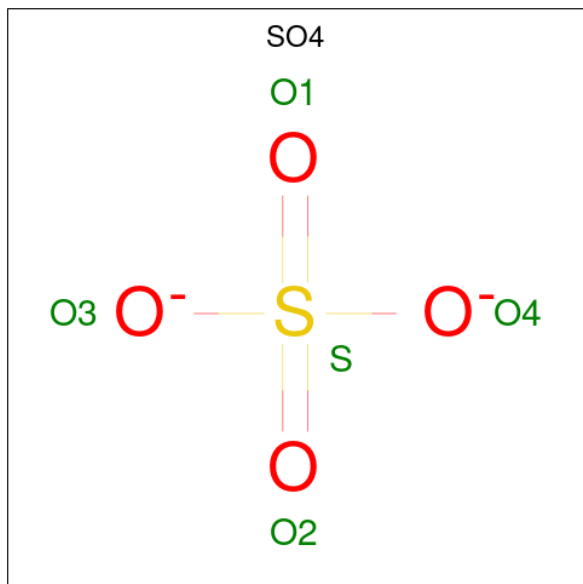
Chain	Residue	Modelled	Actual	Comment	Reference
E	732	ALA	GLY	conflict	UNP Q5UNP4
E	733	HIS	ILE	conflict	UNP Q5UNP4
E	734	LYS	THR	conflict	UNP Q5UNP4
E	786	MSE	MET	modified residue	UNP Q5UNP4
F	1	MSE	MET	modified residue	UNP Q5UNP4
F	7	MSE	MET	modified residue	UNP Q5UNP4
F	46	MSE	MET	modified residue	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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: CL) (formula: Cl).

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

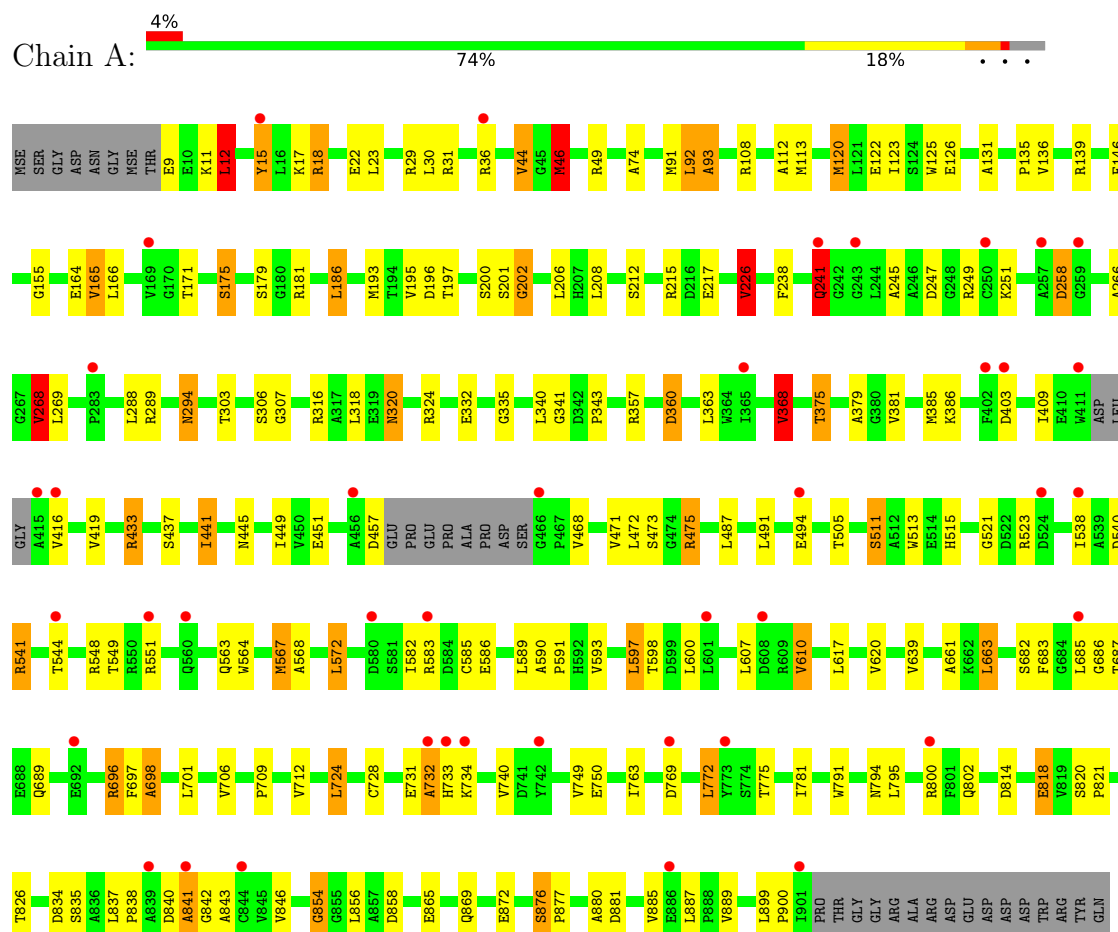
- Molecule 5 is water.

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

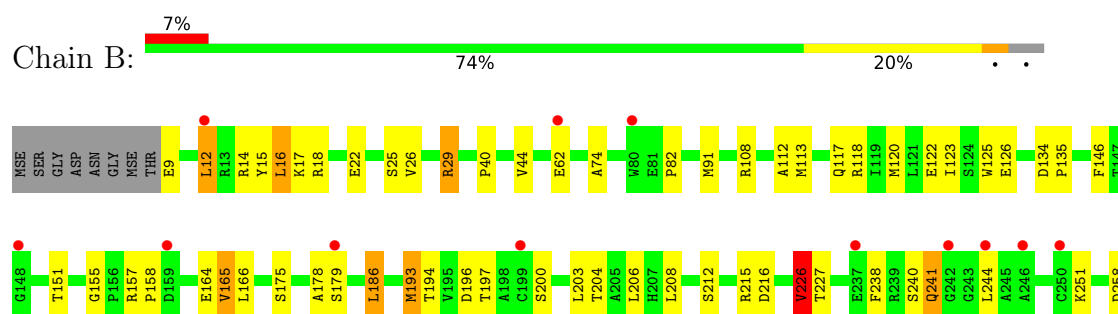
3 Residue-property plots [i](#)

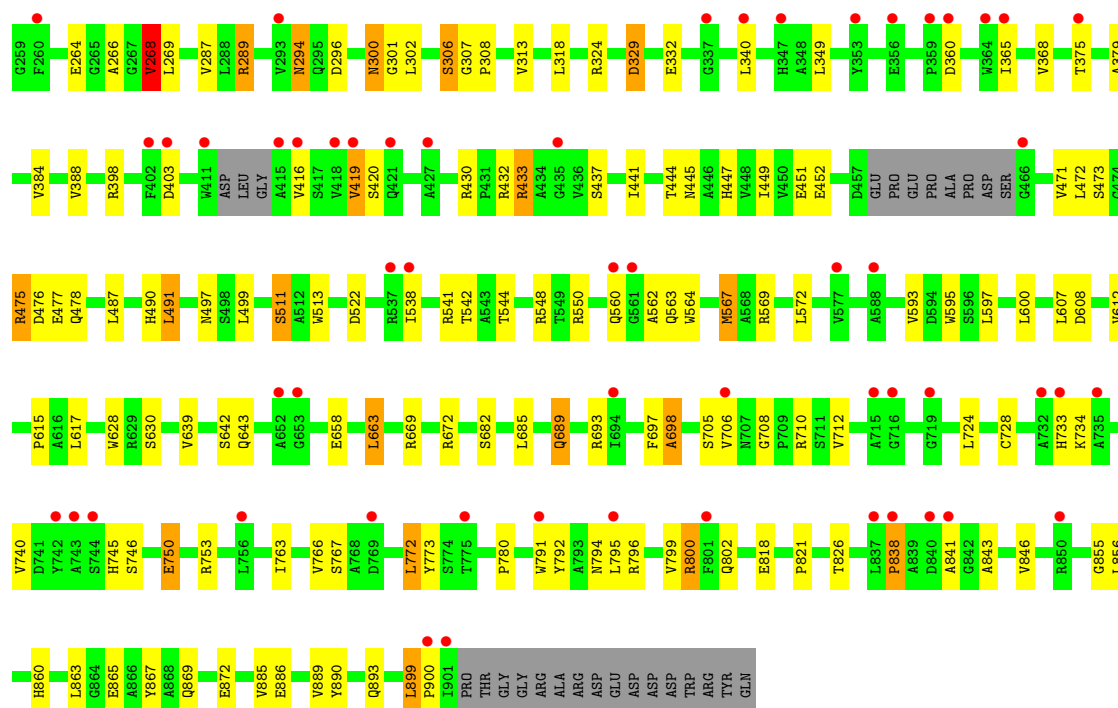
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 6-Deoxyerythronolide B Synthase

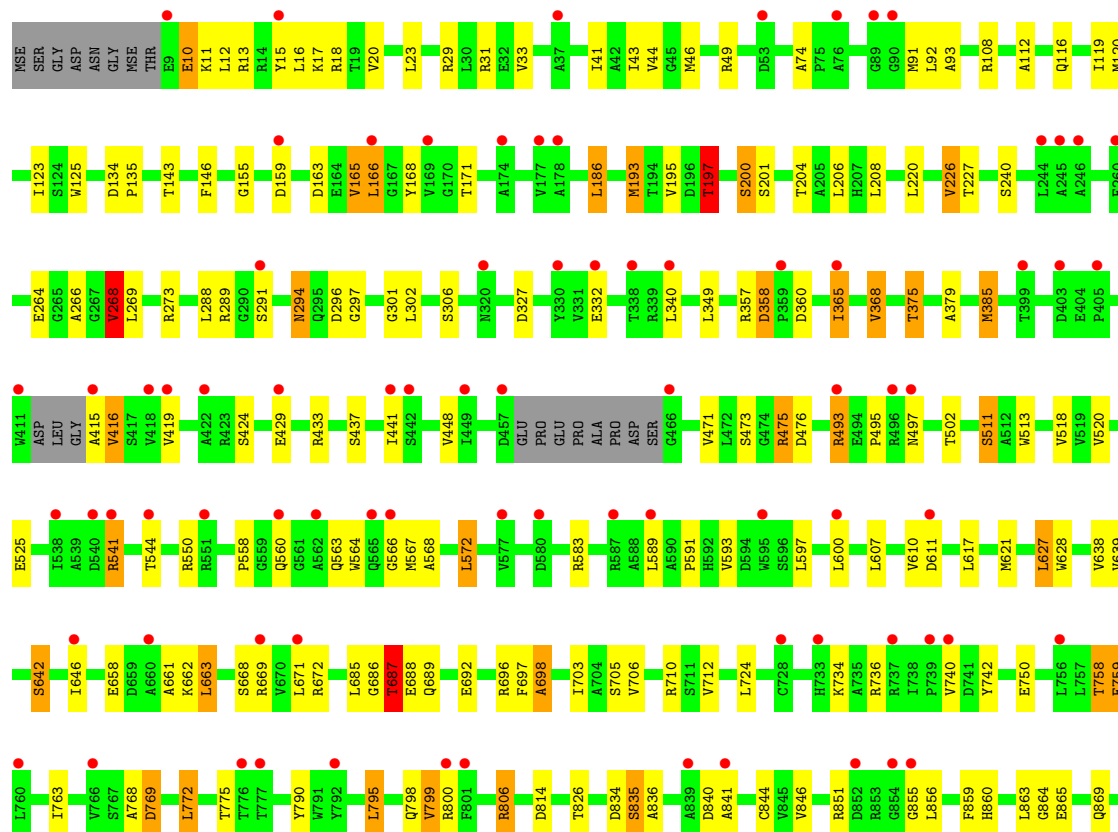
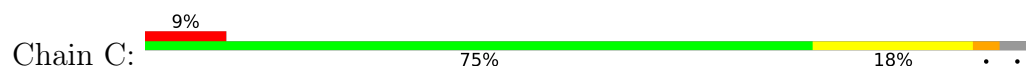


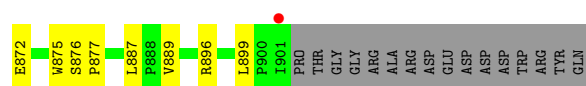
• Molecule 1: 6-Deoxyerythronolide B Synthase



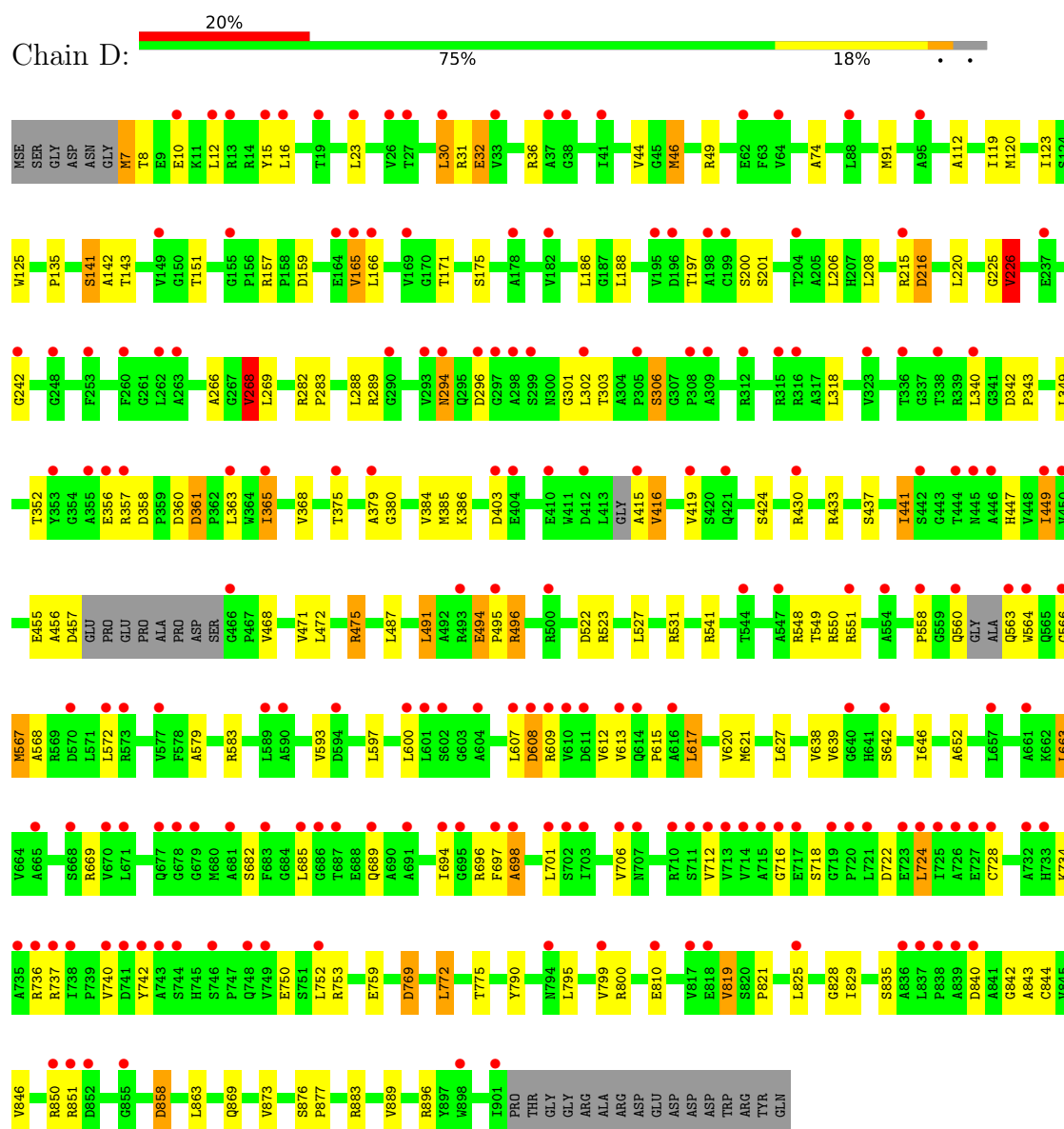


• Molecule 1: 6-Deoxyerythronolide B Synthase

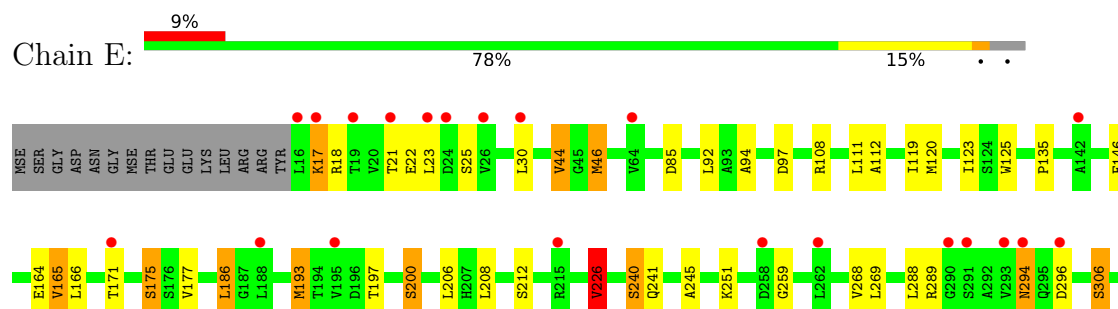


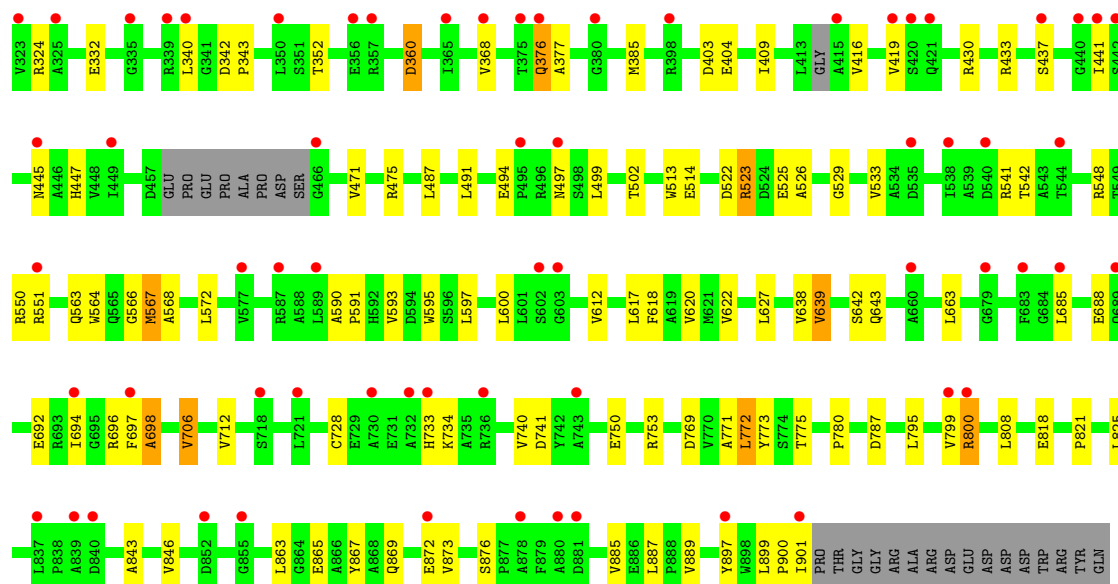


● Molecule 1: 6-Deoxyerythronolide B Synthase

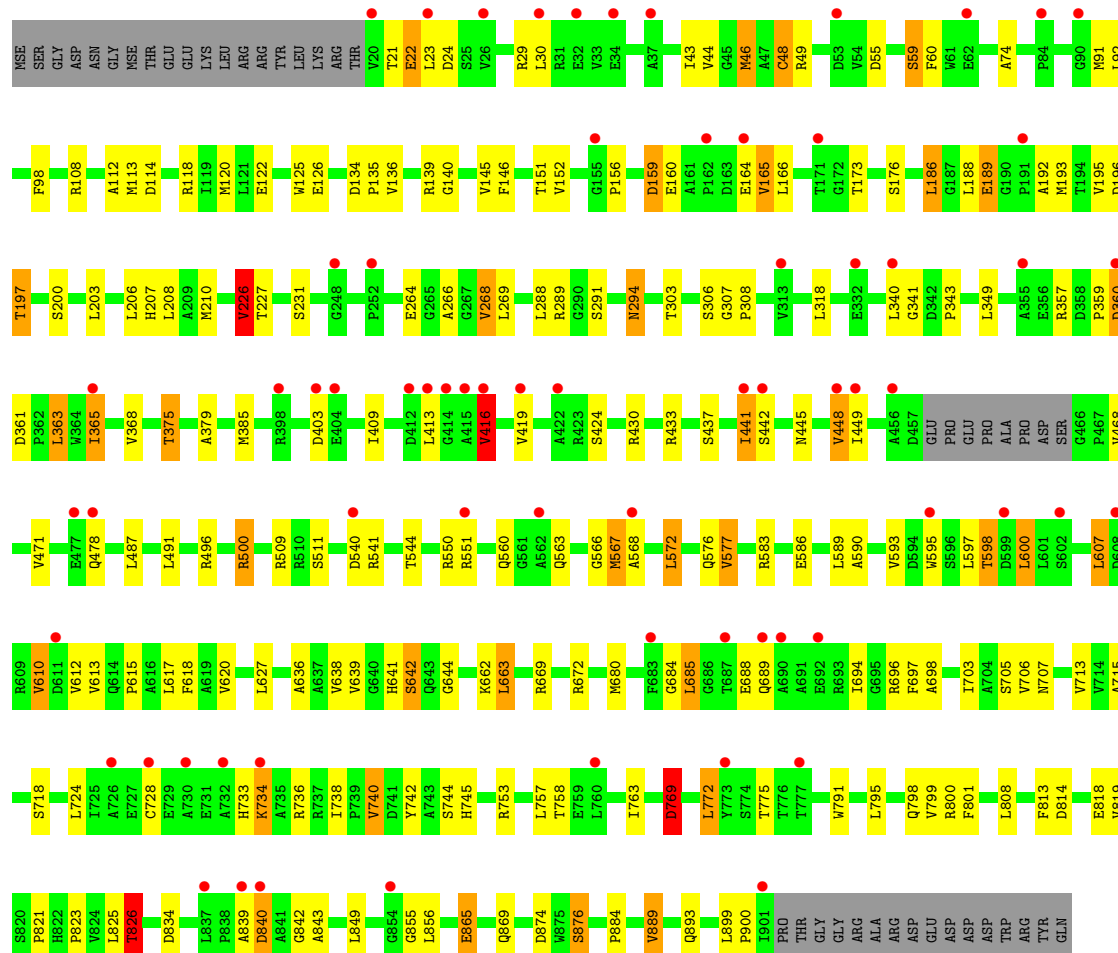


● Molecule 1: 6-Deoxyerythronolide B Synthase





• Molecule 1: 6-Deoxyerythronolide B Synthase



4 Data and refinement statistics

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 48.03 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.73) 99.8 (48.03-2.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.255 0.223 , 0.260	Depositor DCC
R_{free} test set	10395 reflections (5.02%)	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)	0.31 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, 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	0.92	2/6634 (0.0%)	1.02	11/8999 (0.1%)
1	B	0.85	2/6648 (0.0%)	0.95	4/9015 (0.0%)
1	C	0.83	2/6634 (0.0%)	0.95	8/8999 (0.1%)
1	D	0.80	1/6663 (0.0%)	0.94	4/9034 (0.0%)
1	E	0.80	1/6587 (0.0%)	0.93	3/8936 (0.0%)
1	F	0.88	2/6554 (0.0%)	1.00	15/8894 (0.2%)
All	All	0.85	10/39720 (0.0%)	0.97	45/53877 (0.1%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	193	MSE	SE-CE	-6.59	1.75	1.95
1	A	120	MSE	SE-CE	-6.11	1.77	1.95
1	C	193	MSE	SE-CE	-6.04	1.77	1.95
1	B	193	MSE	SE-CE	-5.99	1.77	1.95
1	F	210	MSE	SE-CE	5.79	2.12	1.95
1	D	7	MSE	SE-CE	5.66	2.12	1.95
1	A	46	MSE	SE-CE	-5.57	1.78	1.95
1	F	46	MSE	SE-CE	-5.38	1.79	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	VAL	CA-CB	5.37	1.59	1.53
1	C	385	MSE	SE-CE	-5.35	1.79	1.95

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	226	VAL	CB-CA-C	-7.17	98.05	111.30
1	E	226	VAL	CB-CA-C	-7.08	99.59	110.50
1	C	841	ALA	N-CA-C	-6.92	104.58	113.16
1	A	226	VAL	CB-CA-C	-6.88	98.40	110.71
1	F	738	ILE	N-CA-C	-6.67	102.42	108.95
1	B	226	VAL	CB-CA-C	-6.61	99.27	110.71
1	A	610	VAL	CB-CA-C	-6.33	103.59	112.14
1	D	226	VAL	CB-CA-C	-6.32	100.77	110.50
1	A	843	ALA	N-CA-C	6.30	119.17	110.35
1	A	854	GLY	N-CA-C	-6.21	100.73	112.27
1	F	341	GLY	N-CA-C	6.14	119.92	112.49
1	A	368	VAL	CB-CA-C	-6.09	103.16	112.05
1	A	15	TYR	CA-CB-CG	-5.96	103.18	113.90
1	D	268	VAL	CB-CA-C	-5.91	101.23	110.69
1	D	141	SER	N-CA-C	5.90	120.32	113.18
1	F	416	VAL	N-CA-C	5.88	121.57	109.34
1	B	569	ARG	N-CA-C	-5.87	104.79	111.07
1	C	799	VAL	N-CA-C	5.86	116.51	110.82
1	F	889	VAL	N-CA-CB	-5.85	105.06	112.60
1	F	610	VAL	CB-CA-C	-5.83	104.27	112.14
1	F	48	CYS	N-CA-C	5.79	117.65	108.79
1	C	368	VAL	CB-CA-C	-5.76	100.78	111.79
1	B	843	ALA	N-CA-C	5.71	117.67	110.24
1	C	610	VAL	CB-CA-C	-5.66	104.72	111.97
1	A	241	GLN	N-CA-C	-5.65	103.03	110.43
1	C	768	ALA	N-CA-C	5.62	118.13	109.07
1	F	834	ASP	N-CA-C	-5.59	105.10	111.14
1	F	843	ALA	N-CA-C	5.59	118.59	110.42
1	C	197	THR	N-CA-C	-5.57	104.73	112.03
1	A	781	ILE	N-CA-C	5.43	116.52	108.65
1	A	12	LEU	N-CA-C	-5.42	105.45	111.36
1	F	268	VAL	CB-CA-C	-5.38	101.08	110.71
1	B	268	VAL	CB-CA-C	-5.31	101.20	110.71
1	C	268	VAL	CB-CA-C	-5.31	101.20	110.71
1	F	613	VAL	CB-CA-C	-5.31	105.17	111.81
1	E	404	GLU	N-CA-C	-5.26	102.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	842	GLY	N-CA-C	5.25	125.62	113.18
1	E	44	VAL	CB-CA-C	5.22	116.25	110.62
1	A	268	VAL	CB-CA-C	-5.13	102.75	110.55
1	F	819	VAL	N-CA-C	5.11	111.68	106.21
1	A	341	GLY	N-CA-C	5.08	119.27	112.77
1	C	473	SER	N-CA-C	5.06	116.50	108.96
1	D	30	LEU	N-CA-C	-5.03	105.07	111.11
1	F	613	VAL	N-CA-C	5.03	115.18	110.30
1	F	413	LEU	N-CA-C	-5.01	107.01	112.72

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	95	0
1	B	6534	0	6385	109	0
1	C	6520	0	6359	107	0
1	D	6550	0	6396	97	0
1	E	6474	0	6316	77	0
1	F	6440	0	6274	105	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	578	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 (578) 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:D:294:ASN:C	1:D:294:ASN:HD22	1.81	0.85
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:294:ASN:C	1:A:294:ASN:HD22	1.86	0.83
1:A:193:MSE:HE3	1:A:208:LEU:HD13	1.60	0.83
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:F:294:ASN:C	1:F:294:ASN:HD22	1.92	0.77
1:B:193:MSE:HE3	1:B:208:LEU:HD13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:HA	1:A:258:ASP:HB2	1.64	0.77
1:C:294:ASN:C	1:C:294:ASN:HD22	1.94	0.76
1:F:193:MSE:HE3	1:F:208:LEU:HD13	1.69	0.74
1:B:294:ASN:C	1:B:294:ASN:HD22	1.95	0.73
1:D:701:LEU:HD23	1:D:716:GLY:HA3	1.70	0.72
1:D:620:VAL:HG11	1:D:821:PRO:HG3	1.71	0.72
1:E:294:ASN:HD22	1:E:294:ASN:C	1.98	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:241:GLN:HE21	1:B:241:GLN:C	1.98	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:A:320:ASN:N	1:A:320:ASN:HD22	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:F:206:LEU:C	1:F:206:LEU:HD23	2.20	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:HG22	1:A:197:THR:O	1.94	0.65
1:A:15:TYR:CE1	1:A:18:ARG:HD2	2.32	0.65
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:294:ASN:C	1:D:294:ASN:ND2	2.52	0.63
1:D:361:ASP:OD1	1:D:361:ASP:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:17:LYS:O	1:E:21:THR:OG1	2.08	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:HH11	1:D:475:ARG:HG3	1.65	0.62
1:A:294:ASN:C	1:A:294:ASN:ND2	2.56	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:43:ILE:HG21	1:C:46:MSE:HE3	1.82	0.60
1:C:193:MSE:CE	1:C:208:LEU:HD13	2.29	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:HG22	1:D:197:THR:O	2.02	0.60
1:E:197:THR:O	1:E:197:THR:HG22	2.02	0.60
1:E:901:ILE:C	5:E:1002:HOH:O	2.45	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
1:E:123:ILE:HD12	1:E:268:VAL:HG23	1.86	0.58
1:E:197:THR:HG22	1:E:200:SER:OG	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:ASN:C	1:F:294:ASN:ND2	2.59	0.57
1:F:471:VAL:HG12	5:F:992:HOH:O	2.03	0.57
1:B:289:ARG:HH11	1:B:289:ARG:HG2	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: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:156:PRO:HB2	1:F:160:GLU:HG3	1.87	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:F:576:GLN:O	1:F:577:VAL:C	2.49	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:294:ASN:C	1:B:294:ASN:ND2	2.64	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:HG22	1:C:197:THR:O	2.06	0.55
1:D:32:GLU:OE1	1:D:36:ARG:CZ	2.54	0.55
1:D:197:THR:HG22	1:D:200:SER:OG	2.06	0.55
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:A:268:VAL:C	1:A:269:LEU:HD12	2.31	0.55
1:B:113:MSE:HE2	1:B:118:ARG:HG2	1.89	0.55
1:C:268:VAL:C	1:C:269:LEU:HD12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:D:858:ASP:OD1	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:OD1	1:D:769:ASP:N	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:D:455:GLU:OE1	1:D:455:GLU:HA	2.08	0.53
1:C:294:ASN:C	1:C:294:ASN:ND2	2.66	0.53
1:A:197:THR:O	1:A:197:THR:CG2	2.56	0.53
1:C:15:TYR:CE2	1:E:551:ARG:CZ	2.93	0.52
1:D:775:THR:O	1:D:799:VAL:O	2.27	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:E:294:ASN:C	1:E:294:ASN:ND2	2.66	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:25:SER:O	1:B:29:ARG:HB2	2.09	0.52
1:B:113:MSE:HE2	1:B:118:ARG:CG	2.40	0.52
1:B:697:PHE:O	1:B:698:ALA:C	2.51	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
1:B:215:ARG:O	1:B:216:ASP:HB2	2.09	0.52
1:E:566:GLY:O	1:E:567:MSE:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:697:PHE:O	1:F:698:ALA:C	2.53	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:476:ASP:OD1	1:C:476:ASP:C	2.54	0.51
1:C:206:LEU:HD23	1:C:206:LEU:C	2.35	0.51
1:C:710:ARG:O	1:C:710:ARG:HG2	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:22:GLU:HA	1:E:25:SER:OG	2.11	0.51
1:E:197:THR:O	1:E:197:THR:CG2	2.59	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:N	1:E:688:GLU:OE1	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:A:697:PHE:O	1:A:698:ALA:C	2.54	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: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: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:A:772:LEU:HD12	1:A:772:LEU:C	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:THR:HA	1:F:441:ILE:O	2.12	0.49
1:E:240:SER:C	1:E:241:GLN:O	2.50	0.49
1:B:12:LEU:HD12	1:B:15:TYR:CD2	2.46	0.49
1:C:74:ALA:HA	1:C:91:MSE:HG3	1.94	0.49
1:C:146:PHE:HD2	1:C:193:MSE:HE2	1.77	0.49
1:F:636:ALA:HB3	1:F:813:PHE:HE1	1.78	0.49
1:C:686:GLY:O	1:C:687:THR:C	2.55	0.49
1:F:769:ASP:OD1	1:F:769:ASP:N	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:301:GLY:O	1:D:302:LEU:C	2.55	0.49
1:D:358:ASP:OD2	1:D:360:ASP:HB3	2.13	0.49
1:F:74:ALA:HA	1:F:91:MSE:HG3	1.93	0.49
1:F:500:ARG:HB3	1:F:500:ARG:HH11	1.78	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:E:94:ALA:HB1	1:E:97:ASP:CG	2.38	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:B:197:THR:O	1:B:197:THR:CG2	2.60	0.48
1:C:814:ASP:OD1	1:C:814:ASP:N	2.45	0.48
1:B:125:TRP:CE2	1:B:135:PRO:HG2	2.49	0.48
1:C:611:ASP:HA	1:C:668:SER:HB2	1.94	0.48
1:C:627:LEU:HD22	1:C:859:PHE:CE2	2.49	0.48
1:D:357:ARG:HB2	1:D:415:ALA:HB2	1.95	0.48
1:D:522:ASP:OD1	1:D:522:ASP:C	2.56	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: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
1:A:307:GLY:HA3	5:A:1037:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:268:VAL:C	1:E:269:LEU:HD12	2.39	0.48
1:F:728:CYS:O	1:F:733:HIS:N	2.39	0.48
1:D:200:SER:O	1:D:201:SER:C	2.56	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:A:837:LEU:O	1:A:838:PRO:C	2.57	0.47
1:B:197:THR:HG23	1:B:444:THR:HB	1.96	0.47
1:A:186:LEU:HD23	1:A:186:LEU:N	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:D:386:LYS:NZ	5:D:1001:HOH:O	2.39	0.47
1:F:641:HIS:O	1:F:642:SER:C	2.57	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:F:375:THR:HG23	1:F:379:ALA:N	2.29	0.47
1:F:662:LYS:O	1:F:663:LEU:C	2.58	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

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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:B:134:ASP:OD1	1:B:134:ASP:C	2.58	0.46
1:C:560:GLN:HE21	2:C:950:ACT:C	2.28	0.46
1:A:475:ARG:HG3	1:A:475:ARG:HH11	1.79	0.46
1:B:560:GLN:NE2	1:B:643:GLN:HE22	2.13	0.46
1:B:708:GLY:C	1:B:802:GLN:NE2	2.74	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:522:ASP:O	1:D:523:ARG:C	2.59	0.46
1:D:863:LEU:HD22	1:D:873:VAL:CG1	2.45	0.46
1:E:522:ASP:O	1:E:523:ARG:C	2.57	0.46
1:F:134:ASP:C	1:F:134:ASP:OD1	2.58	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:E:697:PHE:O	1:E:698:ALA:C	2.59	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:HG2	1:B:710:ARG:O	2.15	0.46
1:E:343:PRO:HA	1:E:409:ILE:HG12	1.98	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: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:HH11	1:D:475:ARG:CG	2.27	0.45
1:E:376:GLN:O	1:E:377:ALA:C	2.59	0.45
1:F:560:GLN:HG2	2:F:950:ACT:H1	1.97	0.45
1:F:740:VAL:HG22	1:F:742:TYR:CE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:THR:HG23	1:E:887:LEU:HD21	1.98	0.45
1:B:157:ARG:O	1:B:158:PRO:C	2.57	0.45
1:D:120:MSE:CE	1:D:123:ILE:HD11	2.46	0.45
1:E:120:MSE:SE	1:E:226:VAL:HG22	2.66	0.45
1:E:206:LEU:HD23	1:E:206:LEU:C	2.42	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:O	1:A:165:VAL:HG13	2.17	0.45
1:A:320:ASN:N	1:A:320:ASN:ND2	2.60	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:C:16:LEU:O	1:C:17:LYS:C	2.58	0.45
1:D:608:ASP:OD1	1:D:608:ASP:N	2.49	0.45
1:E:186:LEU:N	1:E:186:LEU:HD23	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:D:494:GLU:CD	1:D:495:PRO:HD2	2.42	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:C:697:PHE:O	1:C:698:ALA:C	2.59	0.45
1:D:225:GLY:O	1:D:266:ALA:HA	2.17	0.45
1:A:215:ARG:HH12	1:A:217:GLU:CD	2.25	0.45
1:B:705:SER:CB	1:B:799:VAL:HB	2.46	0.45
1:C:11:LYS:C	1:E:551:ARG:NH1	2.75	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:PHE:O	1:E:622:VAL:HG23	2.17	0.44
1:F:589:LEU:O	1:F:590:ALA:C	2.61	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:206:LEU:HD21	1:D:288:LEU:HD13	1.99	0.44
1:D:268:VAL:O	1:D:269:LEU:HD12	2.18	0.44
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:A:318:LEU:HD23	1:A:449:ILE:HD13	2.00	0.44
1:C:566:GLY:O	1:C:567:MSE:C	2.60	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:D:268:VAL:C	1:D:269:LEU:HD12	2.43	0.44
1:F:825:LEU:O	1:F:826:THR:C	2.60	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:752:LEU:O	1:D:753:ARG:C	2.58	0.43
1:E:175:SER:HB3	1:F:196:ASP:OD2	2.17	0.43
1:E:294:ASN:ND2	1:E:445:ASN:HB2	2.33	0.43
1:F:294:ASN:HD21	1:F:445:ASN:HB2	1.83	0.43
1:A:44:VAL:HG13	1:A:131:ALA:HB1	2.00	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: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:30:LEU:HD13	1:A:30:LEU:C	2.44	0.43
1:A:201:SER:O	1:A:202:GLY:C	2.60	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:C:834:ASP:O	1:C:835:SER:C	2.61	0.43
1:D:380:GLY:O	1:D:384:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:639:VAL:HG21	1:F:808:LEU:HD11	1.99	0.43
1:B:522:ASP:C	1:B:522:ASP:OD1	2.60	0.43
1:C:875:TRP:O	1:C:876:SER:C	2.62	0.43
1:D:151:THR:HG23	1:D:151:THR:O	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:A:92:LEU:O	1:A:93:ALA:C	2.62	0.43
1:A:585:CYS:O	1:A:586:GLU:C	2.62	0.43
1:B:689:GLN:HE22	1:B:693:ARG:NH1	2.16	0.43
1:B:772:LEU:C	1:B:772:LEU:CD1	2.92	0.43
1:B:772:LEU:C	1:B:772:LEU:HD12	2.44	0.43
1:F:46:MSE:HE2	1:F:269:LEU:CD1	2.49	0.43
1:F:865:GLU:O	1:F:869:GLN:HG3	2.18	0.43
1:A:206:LEU:C	1:A:206:LEU:HD23	2.44	0.43
1:A:728:CYS:O	1:A:732:ALA:N	2.52	0.43
1:C:790:TYR:CD1	1:C:790:TYR:C	2.97	0.43
1:D:10:GLU:OE1	1:D:10:GLU:N	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: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:D:697:PHE:O	1:D:698:ALA:C	2.61	0.43
1:F:125:TRP:CE2	1:F:135:PRO:HG2	2.54	0.43
1:B:203:LEU:O	1:B:204:THR:C	2.61	0.42
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:B:268:VAL:C	1:B:269:LEU:HD12	2.44	0.42
1:C:628:TRP:CZ3	1:C:863:LEU:HD23	2.54	0.42
1:D:157:ARG:C	1:D:159:ASP:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ALA:O	1:A:881:ASP:HB2	2.20	0.42
1:B:476:ASP:OD1	1:B:476:ASP:C	2.62	0.42
1:B:663:LEU:HD11	1:B:791:TRP:CE2	2.55	0.42
1:B:689:GLN:HE21	1:B:689:GLN:HA	1.84	0.42
1:C:12:LEU:O	1:C:13:ARG:C	2.62	0.42
1:E:529:GLY:O	1:E:533:VAL:HG23	2.20	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:A:686:GLY:O	1:A:687:THR:C	2.63	0.42
1:B:294:ASN:HD21	1:B:445:ASN:HB2	1.85	0.42
1:C:662:LYS:O	1:C:663:LEU:C	2.62	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
1:F:48:CYS:SG	1:F:385:MSE:HE1	2.60	0.42
1:F:566:GLY:O	1:F:567:MSE:C	2.63	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:A:818:GLU:OE1	1:A:820:SER:OG	2.29	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:C:120:MSE:CE	1:C:266:ALA:HB1	2.50	0.41
1:C:301:GLY:O	1:C:302:LEU:C	2.62	0.41
1:E:863:LEU:HD22	1:E:873:VAL:CG1	2.49	0.41
1:F:59:SER:O	1:F:60:PHE:C	2.60	0.41
1:A:375:THR:HG22	1:A:379:ALA:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:876:SER:HB2	1:D:877:PRO:HD3	2.02	0.41
1:F:55:ASP:C	1:F:55:ASP:OD1	2.63	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:206:LEU:C	1:F:206:LEU:CD2	2.90	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:D:828:GLY:O	1:D:829:ILE:C	2.64	0.41
1:E:120:MSE:HE3	1:E:226:VAL:HG22	2.01	0.41
1:F:113:MSE:HE2	1:F:118:ARG:HG2	2.03	0.41
1:D:790:TYR:CD1	1:D:790:TYR:C	2.99	0.41
1:F:318:LEU:HD23	1:F:449:ILE:HD13	2.02	0.41
1:A:212:SER:OG	1:A:217:GLU:OE1	2.34	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
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:247:ASP:HB2	1:A:251:LYS:HZ1	1.86	0.41
1:A:582:ILE:HG23	1:A:597:LEU:HD13	2.03	0.41
1:B:16:LEU:O	1:B:17:LYS:C	2.63	0.41
1:B:120:MSE:SE	1:B:226:VAL:HG22	2.70	0.41
1:B:628:TRP:CZ3	1:B:863:LEU:HD23	2.56	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: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:E:639:VAL:CG2	1:E:808:LEU:HD11	2.50	0.41
1:F:685:LEU:HD22	1:F:689:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:744:SER:HB2	1:F:745:HIS:CD2	2.56	0.41
1:F:856:LEU:HD23	1:F:856:LEU:HA	1.92	0.41
1:A:590:ALA:N	1:A:591:PRO:HD2	2.36	0.41
1:B:301:GLY:O	1:B:302:LEU:C	2.64	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:514:GLU:HB2	5:E:1012:HOH:O	2.21	0.41
1:E:787:ASP:OD1	1:E:787:ASP:C	2.64	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:750:GLU:OE2	1:B:792:TYR:OH	2.33	0.40
1:B:899:LEU:HA	1:B:900:PRO:HD3	1.87	0.40
1:C:200:SER:O	1:C:201:SER:C	2.64	0.40
1:D:819:VAL:O	1:D:819:VAL:HG12	2.21	0.40
1:A:749:VAL:O	1:A:749:VAL:HG12	2.20	0.40
1:C:688:GLU:O	1:C:692:GLU:CG	2.66	0.40
1:C:806:ARG:CZ	1:C:806:ARG:HB3	2.51	0.40
1:D:850:ARG:CG	1:D:851:ARG:N	2.85	0.40
1:F:874:ASP:OD1	1:F:874:ASP:C	2.64	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:D:494:GLU:HG3	1:D:496:ARG:CB	2.52	0.40
1:F:359:PRO:O	1:F:360:ASP:C	2.63	0.40
1:A:9:GLU:C	1:A:11:LYS:N	2.79	0.40
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.97	0.40
1:A:838:PRO:HB2	1:A:841:ALA:HB3	2.04	0.40
1:B:491:LEU:HD12	1:B:491:LEU:HA	1.90	0.40
1:C:93:ALA:N	5:C:981:HOH:O	2.55	0.40
1:D:566:GLY:O	1:D:567:MSE:C	2.64	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	876/917 (96%)	823 (94%)	43 (5%)	10 (1%)	11	20
1	B	876/917 (96%)	813 (93%)	55 (6%)	8 (1%)	14	26
1	C	876/917 (96%)	796 (91%)	69 (8%)	11 (1%)	9	16
1	D	876/917 (96%)	808 (92%)	58 (7%)	10 (1%)	11	20
1	E	871/917 (95%)	795 (91%)	65 (8%)	11 (1%)	9	16
1	F	870/917 (95%)	795 (91%)	61 (7%)	14 (2%)	7	13
All	All	5245/5502 (95%)	4830 (92%)	351 (7%)	64 (1%)	10	19

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
1	C	758	THR
1	C	769	ASP
1	C	855	GLY
1	D	698	ALA
1	E	360	ASP
1	E	567	MSE

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

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	647/668 (97%)	551 (85%)	96 (15%)	3	4
1	B	650/668 (97%)	568 (87%)	82 (13%)	4	7
1	C	647/668 (97%)	564 (87%)	83 (13%)	4	7
1	D	652/668 (98%)	571 (88%)	81 (12%)	4	8
1	E	643/668 (96%)	576 (90%)	67 (10%)	7	13
1	F	638/668 (96%)	556 (87%)	82 (13%)	4	7
All	All	3877/4008 (97%)	3386 (87%)	491 (13%)	4	7

All (491) 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	22	GLU
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
1	A	186	LEU
1	A	195	VAL
1	A	226	VAL
1	A	241	GLN
1	A	249	ARG

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Mol	Chain	Res	Type
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	324	ARG
1	A	332	GLU
1	A	340	LEU
1	A	357	ARG
1	A	360	ASP
1	A	363	LEU
1	A	368	VAL
1	A	375	THR
1	A	419	VAL
1	A	433	ARG
1	A	437	SER
1	A	441	ILE
1	A	457	ASP
1	A	468	VAL
1	A	471	VAL
1	A	472	LEU
1	A	475	ARG
1	A	487	LEU
1	A	494	GLU
1	A	511	SER
1	A	523	ARG
1	A	538	ILE
1	A	540	ASP
1	A	541	ARG
1	A	544	THR
1	A	548	ARG
1	A	549	THR
1	A	551	ARG
1	A	563	GLN
1	A	572	LEU
1	A	583	ARG
1	A	593	VAL
1	A	597	LEU
1	A	600	LEU
1	A	607	LEU
1	A	610	VAL

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Mol	Chain	Res	Type
1	A	617	LEU
1	A	639	VAL
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	740	VAL
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	846	VAL
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	9	GLU
1	B	12	LEU
1	B	14	ARG
1	B	16	LEU
1	B	18	ARG
1	B	29	ARG
1	B	44	VAL
1	B	62	GLU
1	B	151	THR
1	B	165	VAL

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Mol	Chain	Res	Type
1	B	166	LEU
1	B	179	SER
1	B	186	LEU
1	B	206	LEU
1	B	212	SER
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	332	GLU
1	B	340	LEU
1	B	360	ASP
1	B	368	VAL
1	B	419	VAL
1	B	430	ARG
1	B	433	ARG
1	B	441	ILE
1	B	472	LEU
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	538	ILE
1	B	541	ARG
1	B	542	THR
1	B	544	THR
1	B	548	ARG
1	B	550	ARG
1	B	563	GLN
1	B	572	LEU
1	B	593	VAL
1	B	597	LEU
1	B	600	LEU
1	B	607	LEU

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Mol	Chain	Res	Type
1	B	608	ASP
1	B	617	LEU
1	B	630	SER
1	B	639	VAL
1	B	658	GLU
1	B	663	LEU
1	B	682	SER
1	B	685	LEU
1	B	689	GLN
1	B	706	VAL
1	B	712	VAL
1	B	724	LEU
1	B	734	LYS
1	B	740	VAL
1	B	746	SER
1	B	750	GLU
1	B	753	ARG
1	B	763	ILE
1	B	772	LEU
1	B	794	ASN
1	B	795	LEU
1	B	800	ARG
1	B	818	GLU
1	B	826	THR
1	B	846	VAL
1	B	872	GLU
1	B	885	VAL
1	B	886	GLU
1	B	889	VAL
1	B	899	LEU
1	C	10	GLU
1	C	18	ARG
1	C	20	VAL
1	C	23	LEU
1	C	29	ARG
1	C	31	ARG
1	C	33	VAL
1	C	41	ILE
1	C	44	VAL
1	C	49	ARG
1	C	92	LEU
1	C	159	ASP

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Mol	Chain	Res	Type
1	C	165	VAL
1	C	166	LEU
1	C	171	THR
1	C	186	LEU
1	C	197	THR
1	C	200	SER
1	C	226	VAL
1	C	240	SER
1	C	268	VAL
1	C	289	ARG
1	C	294	ASN
1	C	327	ASP
1	C	332	GLU
1	C	340	LEU
1	C	357	ARG
1	C	358	ASP
1	C	360	ASP
1	C	365	ILE
1	C	368	VAL
1	C	375	THR
1	C	419	VAL
1	C	424	SER
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	563	GLN
1	C	572	LEU
1	C	583	ARG
1	C	593	VAL
1	C	597	LEU
1	C	600	LEU
1	C	607	LEU
1	C	617	LEU
1	C	627	LEU
1	C	639	VAL

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Mol	Chain	Res	Type
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	763	ILE
1	C	769	ASP
1	C	772	LEU
1	C	775	THR
1	C	795	LEU
1	C	800	ARG
1	C	806	ARG
1	C	826	THR
1	C	844	CYS
1	C	846	VAL
1	C	851	ARG
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	23	LEU
1	D	30	LEU
1	D	31	ARG
1	D	32	GLU
1	D	44	VAL
1	D	46	MSE
1	D	49	ARG
1	D	165	VAL
1	D	166	LEU
1	D	171	THR

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Mol	Chain	Res	Type
1	D	175	SER
1	D	226	VAL
1	D	268	VAL
1	D	289	ARG
1	D	294	ASN
1	D	306	SER
1	D	340	LEU
1	D	352	THR
1	D	356	GLU
1	D	361	ASP
1	D	365	ILE
1	D	368	VAL
1	D	419	VAL
1	D	424	SER
1	D	430	ARG
1	D	433	ARG
1	D	441	ILE
1	D	449	ILE
1	D	468	VAL
1	D	471	VAL
1	D	472	LEU
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

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Mol	Chain	Res	Type
1	D	685	LEU
1	D	689	GLN
1	D	696	ARG
1	D	706	VAL
1	D	712	VAL
1	D	718	SER
1	D	724	LEU
1	D	734	LYS
1	D	736	ARG
1	D	740	VAL
1	D	750	GLU
1	D	759	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	846	VAL
1	D	858	ASP
1	D	869	GLN
1	D	883	ARG
1	D	889	VAL
1	D	896	ARG
1	E	17	LYS
1	E	18	ARG
1	E	23	LEU
1	E	30	LEU
1	E	44	VAL
1	E	46	MSE
1	E	85	ASP
1	E	92	LEU
1	E	165	VAL
1	E	166	LEU
1	E	171	THR
1	E	186	LEU
1	E	200	SER
1	E	212	SER
1	E	226	VAL
1	E	240	SER

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Mol	Chain	Res	Type
1	E	251	LYS
1	E	289	ARG
1	E	294	ASN
1	E	306	SER
1	E	324	ARG
1	E	332	GLU
1	E	340	LEU
1	E	352	THR
1	E	360	ASP
1	E	368	VAL
1	E	419	VAL
1	E	430	ARG
1	E	433	ARG
1	E	441	ILE
1	E	471	VAL
1	E	487	LEU
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
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	694	ILE
1	E	696	ARG
1	E	706	VAL
1	E	712	VAL
1	E	734	LYS
1	E	740	VAL
1	E	741	ASP
1	E	750	GLU
1	E	753	ARG

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Mol	Chain	Res	Type
1	E	769	ASP
1	E	772	LEU
1	E	795	LEU
1	E	800	ARG
1	E	846	VAL
1	E	872	GLU
1	E	876	SER
1	E	885	VAL
1	E	889	VAL
1	F	29	ARG
1	F	30	LEU
1	F	44	VAL
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	186	LEU
1	F	189	GLU
1	F	195	VAL
1	F	197	THR
1	F	226	VAL
1	F	231	SER
1	F	268	VAL
1	F	289	ARG
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	375	THR
1	F	419	VAL
1	F	424	SER
1	F	430	ARG
1	F	433	ARG

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Mol	Chain	Res	Type
1	F	437	SER
1	F	441	ILE
1	F	448	VAL
1	F	468	VAL
1	F	487	LEU
1	F	491	LEU
1	F	496	ARG
1	F	500	ARG
1	F	511	SER
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	593	VAL
1	F	597	LEU
1	F	598	THR
1	F	600	LEU
1	F	607	LEU
1	F	610	VAL
1	F	617	LEU
1	F	627	LEU
1	F	663	LEU
1	F	685	LEU
1	F	688	GLU
1	F	694	ILE
1	F	696	ARG
1	F	706	VAL
1	F	718	SER
1	F	724	LEU
1	F	734	LYS
1	F	736	ARG
1	F	740	VAL
1	F	763	ILE
1	F	769	ASP
1	F	772	LEU
1	F	775	THR
1	F	795	LEU
1	F	800	ARG

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Mol	Chain	Res	Type
1	F	814	ASP
1	F	818	GLU
1	F	826	THR
1	F	865	GLU
1	F	876	SER
1	F	889	VAL
1	F	899	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	294	ASN
1	A	311	GLN
1	A	320	ASN
1	A	371	ASN
1	A	376	GLN
1	A	445	ASN
1	A	483	GLN
1	A	515	HIS
1	A	689	GLN
1	A	748	GLN
1	A	779	GLN
1	A	802	GLN
1	B	241	GLN
1	B	294	ASN
1	B	300	ASN
1	B	376	GLN
1	B	445	ASN
1	B	483	GLN
1	B	497	ASN
1	B	560	GLN
1	B	643	GLN
1	B	689	GLN
1	B	807	GLN
1	B	860	HIS
1	C	35	HIS
1	C	241	GLN
1	C	294	ASN
1	C	295	GLN
1	C	300	ASN
1	C	320	ASN

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Mol	Chain	Res	Type
1	C	334	HIS
1	C	371	ASN
1	C	376	GLN
1	C	478	GLN
1	C	483	GLN
1	C	560	GLN
1	C	592	HIS
1	C	643	GLN
1	C	794	ASN
1	D	35	HIS
1	D	133	HIS
1	D	272	GLN
1	D	294	ASN
1	D	311	GLN
1	D	376	GLN
1	D	408	GLN
1	D	445	ASN
1	D	483	GLN
1	D	497	ASN
1	D	560	GLN
1	D	689	GLN
1	D	748	GLN
1	D	807	GLN
1	E	294	ASN
1	E	334	HIS
1	E	483	GLN
1	E	490	HIS
1	E	497	ASN
1	E	515	HIS
1	E	748	GLN
1	F	35	HIS
1	F	241	GLN
1	F	294	ASN
1	F	334	HIS
1	F	376	GLN
1	F	483	GLN
1	F	490	HIS
1	F	560	GLN
1	F	643	GLN
1	F	779	GLN
1	F	798	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	SO4	B	975	-	4,4,4	0.17	0	6,6,6	0.25	0
2	ACT	A	950	-	3,3,3	0.90	0	3,3,3	1.62	1 (33%)
2	ACT	F	950	-	3,3,3	0.91	0	3,3,3	1.90	1 (33%)
2	ACT	D	950	-	3,3,3	0.80	0	3,3,3	2.13	2 (66%)
3	SO4	E	975	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	F	975	-	4,4,4	0.27	0	6,6,6	0.41	0
3	SO4	A	975	-	4,4,4	0.26	0	6,6,6	0.20	0
2	ACT	E	950	-	3,3,3	0.88	0	3,3,3	0.87	0
3	SO4	C	975	-	4,4,4	0.27	0	6,6,6	0.25	0
2	ACT	C	950	-	3,3,3	0.82	0	3,3,3	1.24	0
2	ACT	B	950	-	3,3,3	0.75	0	3,3,3	1.62	1 (33%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	950	ACT	OXT-C-O	-2.67	112.12	122.03
2	D	950	ACT	OXT-C-CH3	2.61	126.00	115.05
2	D	950	ACT	OXT-C-O	-2.59	112.42	122.03
2	A	950	ACT	OXT-C-O	-2.06	114.39	122.03
2	B	950	ACT	OXT-C-CH3	2.05	123.64	115.05

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
3	B	975	SO4	1	0
2	F	950	ACT	1	0
2	D	950	ACT	1	0
3	E	975	SO4	1	0
2	E	950	ACT	1	0
2	C	950	ACT	4	0
2	B	950	ACT	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	867/917 (94%)	0.72	41 (4%)	36 36	34, 67, 80, 94	0
1	B	867/917 (94%)	0.97	67 (7%)	19 19	46, 67, 80, 93	0
1	C	867/917 (94%)	0.93	81 (9%)	14 14	47, 67, 80, 93	0
1	D	868/917 (94%)	1.36	187 (21%)	2 2	48, 67, 80, 93	0
1	E	862/917 (94%)	0.99	85 (9%)	13 13	48, 67, 81, 93	0
1	F	859/917 (93%)	0.94	68 (7%)	18 19	48, 67, 80, 93	0
All	All	5190/5502 (94%)	0.98	529 (10%)	12 12	34, 67, 80, 94	0

All (529) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	20	VAL	11.0
1	E	16	LEU	6.4
1	D	716	GLY	5.7
1	D	495	PRO	5.6
1	D	743	ALA	4.9
1	D	720	PRO	4.9
1	B	901	ILE	4.8
1	D	711	SER	4.7
1	D	840	ASP	4.6
1	D	551	ARG	4.6
1	C	901	ILE	4.5
1	B	12	LEU	4.4
1	A	769	ASP	4.3
1	F	901	ILE	4.3
1	B	841	ALA	4.2
1	D	732	ALA	4.1
1	D	742	TYR	4.0
1	E	551	ARG	4.0
1	D	714	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	560	GLN	4.0
1	E	901	ILE	3.9
1	D	560	GLN	3.9
1	F	692	GLU	3.8
1	F	456	ALA	3.8
1	D	668	SER	3.7
1	D	715	ALA	3.7
1	D	30	LEU	3.7
1	D	23	LEU	3.7
1	D	298	ALA	3.7
1	D	681	ALA	3.7
1	D	691	ALA	3.7
1	E	733	HIS	3.6
1	E	415	ALA	3.6
1	B	421	GLN	3.6
1	C	359	PRO	3.6
1	D	640	GLY	3.6
1	E	290	GLY	3.6
1	D	728	CYS	3.6
1	A	403	ASP	3.5
1	D	356	GLU	3.5
1	D	16	LEU	3.5
1	D	683	PHE	3.5
1	E	732	ALA	3.4
1	E	881	ASP	3.4
1	D	657	LEU	3.4
1	C	90	GLY	3.4
1	D	686	GLY	3.4
1	D	601	LEU	3.4
1	C	441	ILE	3.4
1	D	697	PHE	3.4
1	F	403	ASP	3.3
1	B	742	TYR	3.3
1	C	15	TYR	3.3
1	D	748	GLN	3.3
1	E	683	PHE	3.3
1	D	375	THR	3.3
1	D	837	LEU	3.3
1	F	30	LEU	3.3
1	F	854	GLY	3.3
1	D	706	VAL	3.3
1	D	740	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	670	VAL	3.3
1	D	340	LEU	3.2
1	D	685	LEU	3.2
1	A	241	GLN	3.2
1	D	661	ALA	3.2
1	E	441	ILE	3.2
1	A	734	LYS	3.2
1	C	756	LEU	3.2
1	D	717	GLU	3.2
1	C	839	ALA	3.2
1	C	841	ALA	3.2
1	B	419	VAL	3.2
1	D	721	LEU	3.2
1	C	9	GLU	3.1
1	E	19	THR	3.1
1	C	415	ALA	3.1
1	E	497	ASN	3.1
1	D	27	THR	3.1
1	F	415	ALA	3.1
1	C	541	ARG	3.1
1	B	838	PRO	3.1
1	C	595	TRP	3.1
1	F	602	SER	3.1
1	D	421	GLN	3.1
1	C	422	ALA	3.1
1	D	694	ILE	3.1
1	A	411	TRP	3.1
1	B	537	ARG	3.1
1	D	724	LEU	3.0
1	E	340	LEU	3.0
1	E	21	THR	3.0
1	E	495	PRO	3.0
1	B	538	ILE	3.0
1	D	839	ALA	3.0
1	A	733	HIS	3.0
1	E	296	ASP	3.0
1	C	854	GLY	3.0
1	D	338	THR	3.0
1	F	726	ALA	3.0
1	D	602	SER	3.0
1	F	34	GLU	3.0
1	D	838	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	353	TYR	3.0
1	D	749	VAL	3.0
1	E	294	ASN	2.9
1	D	616	ALA	2.9
1	C	411	TRP	2.9
1	C	560	GLN	2.9
1	E	339	ARG	2.9
1	F	551	ARG	2.9
1	D	608	ASP	2.9
1	B	415	ALA	2.9
1	D	302	LEU	2.9
1	D	12	LEU	2.9
1	A	551	ARG	2.9
1	B	411	TRP	2.9
1	D	199	CYS	2.9
1	B	756	LEU	2.9
1	D	26	VAL	2.9
1	B	365	ILE	2.8
1	F	728	CYS	2.8
1	C	246	ALA	2.8
1	D	563	GLN	2.8
1	E	365	ILE	2.8
1	E	17	LYS	2.8
1	B	840	ASP	2.8
1	D	198	ALA	2.8
1	D	309	ALA	2.8
1	E	325	ALA	2.8
1	D	169	VAL	2.8
1	A	560	GLN	2.8
1	A	466	GLY	2.8
1	D	735	ALA	2.8
1	D	316	ARG	2.8
1	C	855	GLY	2.8
1	D	600	LEU	2.8
1	D	695	GLY	2.8
1	D	611	ASP	2.8
1	A	886	GLU	2.8
1	D	323	VAL	2.8
1	F	595	TRP	2.7
1	D	10	GLU	2.7
1	D	296	ASP	2.7
1	D	726	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	404	GLU	2.7
1	F	839	ALA	2.7
1	C	497	ASN	2.7
1	D	164	GLU	2.7
1	D	710	ARG	2.7
1	E	419	VAL	2.7
1	E	540	ASP	2.7
1	D	901	ILE	2.7
1	D	746	SER	2.7
1	A	415	ALA	2.7
1	D	37	ALA	2.7
1	D	590	ALA	2.7
1	E	293	VAL	2.7
1	B	360	ASP	2.7
1	C	671	LEU	2.7
1	D	297	GLY	2.7
1	D	95	ALA	2.7
1	D	713	VAL	2.7
1	D	817	VAL	2.7
1	F	730	ALA	2.7
1	B	359	PRO	2.7
1	D	594	ASP	2.7
1	F	252	PRO	2.7
1	D	738	ILE	2.6
1	B	250	CYS	2.6
1	C	733	HIS	2.6
1	D	38	GLY	2.6
1	D	566	GLY	2.6
1	D	707	ASN	2.6
1	B	652	ALA	2.6
1	D	577	VAL	2.6
1	F	732	ALA	2.6
1	D	558	PRO	2.6
1	F	171	THR	2.6
1	A	608	ASP	2.6
1	C	540	ASP	2.6
1	D	689	GLN	2.6
1	F	608	ASP	2.6
1	F	689	GLN	2.6
1	C	538	ILE	2.6
1	D	449	ILE	2.6
1	D	13	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	494	GLU	2.6
1	D	719	GLY	2.6
1	F	248	GLY	2.6
1	C	320	ASN	2.6
1	D	64	VAL	2.6
1	D	293	VAL	2.6
1	E	420	SER	2.6
1	C	580	ASP	2.6
1	D	403	ASP	2.6
1	F	611	ASP	2.6
1	D	701	LEU	2.6
1	A	800	ARG	2.6
1	D	493	ARG	2.6
1	D	733	HIS	2.6
1	D	851	ARG	2.6
1	A	839	ALA	2.6
1	D	204	THR	2.6
1	E	840	ASP	2.6
1	C	600	LEU	2.6
1	F	398	ARG	2.6
1	F	734	LYS	2.6
1	B	199	CYS	2.6
1	D	446	ALA	2.6
1	E	26	VAL	2.6
1	D	614	GLN	2.6
1	E	535	ASP	2.5
1	C	365	ILE	2.5
1	E	449	ILE	2.5
1	E	215	ARG	2.5
1	F	332	GLU	2.5
1	B	653	GLY	2.5
1	B	416	VAL	2.5
1	D	836	ALA	2.5
1	E	743	ALA	2.5
1	F	683	PHE	2.5
1	D	19	THR	2.5
1	B	769	ASP	2.5
1	B	340	LEU	2.5
1	B	337	GLY	2.5
1	D	195	VAL	2.5
1	D	355	ALA	2.5
1	C	449	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	551	ARG	2.5
1	D	412	ASP	2.5
1	A	742	TYR	2.5
1	D	679	GLY	2.5
1	E	603	GLY	2.5
1	D	308	PRO	2.5
1	D	253	PHE	2.5
1	F	422	ALA	2.5
1	F	690	ALA	2.5
1	B	375	THR	2.5
1	C	496	ARG	2.5
1	D	357	ARG	2.5
1	D	430	ARG	2.5
1	F	837	LEU	2.5
1	D	404	GLU	2.5
1	D	818	GLU	2.5
1	B	706	VAL	2.5
1	D	547	ALA	2.5
1	E	839	ALA	2.5
1	B	850	ARG	2.4
1	F	23	LEU	2.4
1	E	442	SER	2.4
1	C	53	ASP	2.4
1	E	852	ASP	2.4
1	F	540	ASP	2.4
1	E	335	GLY	2.4
1	A	169	VAL	2.4
1	A	416	VAL	2.4
1	B	260	PHE	2.4
1	B	427	ALA	2.4
1	C	260	PHE	2.4
1	D	698	ALA	2.4
1	F	562	ALA	2.4
1	E	587	ARG	2.4
1	D	825	LEU	2.4
1	A	524	ASP	2.4
1	B	159	ASP	2.4
1	B	403	ASP	2.4
1	A	692	GLU	2.4
1	B	716	GLY	2.4
1	D	305	PRO	2.4
1	A	15	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	743	ALA	2.4
1	D	554	ALA	2.4
1	D	736	ARG	2.4
1	A	365	ILE	2.4
1	A	601	LEU	2.4
1	A	901	ILE	2.4
1	E	171	THR	2.4
1	D	794	ASN	2.4
1	D	442	SER	2.4
1	D	642	SER	2.4
1	D	196	ASP	2.4
1	E	855	GLY	2.4
1	C	587	ARG	2.4
1	C	792	TYR	2.4
1	E	602	SER	2.4
1	D	677	GLN	2.4
1	C	669	ARG	2.4
1	C	766	VAL	2.4
1	D	315	ARG	2.4
1	D	500	ARG	2.4
1	D	610	VAL	2.4
1	D	613	VAL	2.4
1	E	577	VAL	2.4
1	F	26	VAL	2.4
1	F	313	VAL	2.4
1	E	880	ALA	2.4
1	F	355	ALA	2.4
1	C	330	TYR	2.3
1	D	363	LEU	2.3
1	E	685	LEU	2.3
1	F	449	ILE	2.3
1	C	544	THR	2.3
1	D	444	THR	2.3
1	D	687	THR	2.3
1	F	777	THR	2.3
1	B	733	HIS	2.3
1	C	403	ASP	2.3
1	D	852	ASP	2.3
1	F	412	ASP	2.3
1	B	435	GLY	2.3
1	F	90	GLY	2.3
1	D	419	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	368	VAL	2.3
1	A	841	ALA	2.3
1	C	660	ALA	2.3
1	D	604	ALA	2.3
1	F	37	ALA	2.3
1	C	646	ILE	2.3
1	D	365	ILE	2.3
1	C	776	THR	2.3
1	D	445	ASN	2.3
1	D	299	SER	2.3
1	B	242	GLY	2.3
1	B	466	GLY	2.3
1	B	561	GLY	2.3
1	C	89	GLY	2.3
1	D	290	GLY	2.3
1	E	466	GLY	2.3
1	B	402	PHE	2.3
1	D	260	PHE	2.3
1	A	257	ALA	2.3
1	D	262	LEU	2.3
1	D	572	LEU	2.3
1	D	589	LEU	2.3
1	E	23	LEU	2.3
1	E	350	LEU	2.3
1	E	730	ALA	2.3
1	E	538	ILE	2.3
1	C	338	THR	2.3
1	E	375	THR	2.3
1	B	356	GLU	2.3
1	F	477	GLU	2.3
1	D	570	ASP	2.3
1	E	24	ASP	2.3
1	F	162	PRO	2.3
1	F	840	ASP	2.3
1	A	583	ARG	2.3
1	D	737	ARG	2.3
1	B	837	LEU	2.3
1	C	244	LEU	2.3
1	D	415	ALA	2.3
1	B	237	GLU	2.3
1	F	32	GLU	2.3
1	B	900	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	291	SER	2.3
1	D	702	SER	2.3
1	F	84	PRO	2.3
1	E	440	GLY	2.3
1	D	607	LEU	2.3
1	D	752	LEU	2.3
1	E	323	VAL	2.3
1	F	413	LEU	2.3
1	A	732	ALA	2.2
1	C	37	ALA	2.2
1	D	178	ALA	2.2
1	E	544	THR	2.2
1	D	237	GLU	2.2
1	A	773	TYR	2.2
1	D	353	TYR	2.2
1	D	573	ARG	2.2
1	D	850	ARG	2.2
1	E	398	ARG	2.2
1	B	179	SER	2.2
1	F	414	GLY	2.2
1	B	364	TRP	2.2
1	B	577	VAL	2.2
1	C	418	VAL	2.2
1	D	182	VAL	2.2
1	D	799	VAL	2.2
1	E	837	LEU	2.2
1	F	760	LEU	2.2
1	A	844	CYS	2.2
1	B	62	GLU	2.2
1	C	429	GLU	2.2
1	D	15	TYR	2.2
1	D	294	ASN	2.2
1	A	283	PRO	2.2
1	B	744	SER	2.2
1	D	855	GLY	2.2
1	E	380	GLY	2.2
1	E	188	LEU	2.2
1	C	419	VAL	2.2
1	E	64	VAL	2.2
1	A	538	ILE	2.2
1	D	725	ILE	2.2
1	F	365	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	456	ALA	2.2
1	E	878	ALA	2.2
1	A	250	CYS	2.2
1	D	727	GLU	2.2
1	D	312	ARG	2.2
1	D	609	ARG	2.2
1	A	580	ASP	2.2
1	B	148	GLY	2.2
1	E	799	VAL	2.2
1	E	697	PHE	2.2
1	B	246	ALA	2.2
1	D	410	GLU	2.2
1	A	544	THR	2.2
1	E	445	ASN	2.2
1	A	685	LEU	2.2
1	E	721	LEU	2.2
1	F	340	LEU	2.2
1	D	741	ASP	2.2
1	D	744	SER	2.2
1	D	703	ILE	2.2
1	E	195	VAL	2.2
1	E	291	SER	2.2
1	B	347	HIS	2.2
1	C	332	GLU	2.1
1	E	356	GLU	2.1
1	F	164	GLU	2.1
1	D	215	ARG	2.1
1	D	544	THR	2.1
1	E	421	GLN	2.1
1	B	795	LEU	2.1
1	D	166	LEU	2.1
1	A	259	GLY	2.1
1	C	466	GLY	2.1
1	F	155	GLY	2.1
1	D	33	VAL	2.1
1	D	165	VAL	2.1
1	B	588	ALA	2.1
1	B	732	ALA	2.1
1	C	174	ALA	2.1
1	F	62	GLU	2.1
1	C	737	ARG	2.1
1	B	775	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	376	GLN	2.1
1	F	773	TYR	2.1
1	B	418	VAL	2.1
1	C	611	ASP	2.1
1	D	450	VAL	2.1
1	E	258	ASP	2.1
1	A	402	PHE	2.1
1	B	801	PHE	2.1
1	C	442	SER	2.1
1	F	442	SER	2.1
1	D	810	GLU	2.1
1	B	791	TRP	2.1
1	D	564	TRP	2.1
1	D	898	TRP	2.1
1	E	800	ARG	2.1
1	F	687	THR	2.1
1	E	689	GLN	2.1
1	D	242	GLY	2.1
1	C	169	VAL	2.1
1	C	740	VAL	2.1
1	D	712	VAL	2.1
1	F	419	VAL	2.1
1	A	36	ARG	2.1
1	B	715	ALA	2.1
1	C	493	ARG	2.1
1	C	800	ARG	2.1
1	D	379	ALA	2.1
1	E	718	SER	2.1
1	F	568	ALA	2.1
1	C	399	THR	2.1
1	C	777	THR	2.1
1	D	336	THR	2.1
1	C	405	PRO	2.1
1	B	244	LEU	2.1
1	C	760	LEU	2.1
1	E	30	LEU	2.1
1	B	719	GLY	2.1
1	D	155	GLY	2.1
1	D	466	GLY	2.1
1	D	678	GLY	2.1
1	E	694	ILE	2.1
1	B	293	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	416	VAL	2.1
1	E	736	ARG	2.0
1	F	53	ASP	2.0
1	F	360	ASP	2.0
1	F	599	ASP	2.0
1	B	735	ALA	2.0
1	C	76	ALA	2.0
1	C	178	ALA	2.0
1	C	562	ALA	2.0
1	D	263	ALA	2.0
1	D	665	ALA	2.0
1	D	723	GLU	2.0
1	E	142	ALA	2.0
1	E	872	GLU	2.0
1	E	437	SER	2.0
1	C	340	LEU	2.0
1	C	565	GLN	2.0
1	C	589	LEU	2.0
1	E	262	LEU	2.0
1	B	694	ILE	2.0
1	D	41	ILE	2.0
1	E	679	GLY	2.0
1	C	728	CYS	2.0
1	E	897	TYR	2.0
1	C	801	PHE	2.0
1	E	357	ARG	2.0
1	C	159	ASP	2.0
1	C	457	ASP	2.0
1	C	852	ASP	2.0
1	D	62	GLU	2.0
1	C	245	ALA	2.0
1	E	660	ALA	2.0
1	B	80	TRP	2.0
1	C	739	PRO	2.0
1	F	191	PRO	2.0
1	C	166	LEU	2.0
1	D	88	LEU	2.0
1	D	671	LEU	2.0
1	E	589	LEU	2.0
1	F	478	GLN	2.0
1	A	243	GLY	2.0
1	C	566	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	248	GLY	2.0
1	F	441	ILE	2.0
1	C	177	VAL	2.0
1	C	577	VAL	2.0
1	D	149	VAL	2.0
1	F	448	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	975	5/5	0.73	0.15	109,109,109,109	0
3	SO4	E	975	5/5	0.80	0.17	101,101,102,102	5
3	SO4	C	975	5/5	0.82	0.17	84,84,85,86	5
2	ACT	D	950	4/4	0.83	0.18	61,61,61,62	0
4	CL	D	951	1/1	0.83	0.15	90,90,90,90	0
4	CL	F	976	1/1	0.87	0.16	76,76,76,76	0
2	ACT	F	950	4/4	0.88	0.16	44,44,45,45	0
4	CL	C	976	1/1	0.90	0.13	82,82,82,82	0
2	ACT	B	950	4/4	0.92	0.15	50,50,50,50	0
2	ACT	A	950	4/4	0.93	0.15	51,51,51,51	0
4	CL	E	976	1/1	0.93	0.12	70,70,70,70	0
3	SO4	A	975	5/5	0.93	0.18	87,87,88,88	0
2	ACT	E	950	4/4	0.94	0.14	47,48,48,48	0
2	ACT	C	950	4/4	0.94	0.13	54,54,54,54	0
3	SO4	F	975	5/5	0.95	0.19	82,82,83,83	0
4	CL	B	976	1/1	0.98	0.09	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.