Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:57 PM GMT

PDB ID	:	1R3N
Title	:	Crystal structure of beta-alanine synthase from Saccharomyces kluyveri
Authors	:	Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritzsch, D.
Deposited on	:	2003-10-02
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

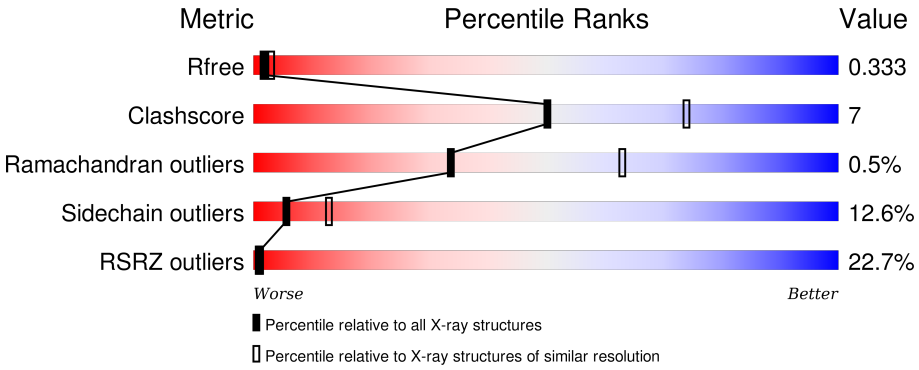
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	13% 73% 19% • 5%
1	B	462	17% 71% 21% • 6%
1	C	462	9% 76% 16% • 5%
1	D	462	21% 75% 17% • 5%
1	E	462	46% 64% 26% 5% 6%

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Mol	Chain	Length	Quality of chain
1	F	462	10% 76% 16% • 5%
1	G	462	46% 65% 24% • 7%
1	H	462	10% 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
3	BIB	E	6502	-	-	-	X
3	BIB	G	8502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27487 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 beta-alanine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	B	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	C	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	D	437	Total	C	N	O	S	0	0	0
			3375	2128	579	652	16			
1	E	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	F	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	G	430	Total	C	N	O	S	0	0	0
			3327	2097	571	643	16			
1	H	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	HIS	-	EXPRESSION TAG	UNP Q96W94
A	457	HIS	-	EXPRESSION TAG	UNP Q96W94
A	458	HIS	-	EXPRESSION TAG	UNP Q96W94
A	459	HIS	-	EXPRESSION TAG	UNP Q96W94
A	460	HIS	-	EXPRESSION TAG	UNP Q96W94
A	461	HIS	-	EXPRESSION TAG	UNP Q96W94
A	462	HIS	-	EXPRESSION TAG	UNP Q96W94
A	463	HIS	-	EXPRESSION TAG	UNP Q96W94
B	456	HIS	-	EXPRESSION TAG	UNP Q96W94
B	457	HIS	-	EXPRESSION TAG	UNP Q96W94
B	458	HIS	-	EXPRESSION TAG	UNP Q96W94
B	459	HIS	-	EXPRESSION TAG	UNP Q96W94
B	460	HIS	-	EXPRESSION TAG	UNP Q96W94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	EXPRESSION TAG	UNP Q96W94
B	462	HIS	-	EXPRESSION TAG	UNP Q96W94
B	463	HIS	-	EXPRESSION TAG	UNP Q96W94
C	456	HIS	-	EXPRESSION TAG	UNP Q96W94
C	457	HIS	-	EXPRESSION TAG	UNP Q96W94
C	458	HIS	-	EXPRESSION TAG	UNP Q96W94
C	459	HIS	-	EXPRESSION TAG	UNP Q96W94
C	460	HIS	-	EXPRESSION TAG	UNP Q96W94
C	461	HIS	-	EXPRESSION TAG	UNP Q96W94
C	462	HIS	-	EXPRESSION TAG	UNP Q96W94
C	463	HIS	-	EXPRESSION TAG	UNP Q96W94
D	456	HIS	-	EXPRESSION TAG	UNP Q96W94
D	457	HIS	-	EXPRESSION TAG	UNP Q96W94
D	458	HIS	-	EXPRESSION TAG	UNP Q96W94
D	459	HIS	-	EXPRESSION TAG	UNP Q96W94
D	460	HIS	-	EXPRESSION TAG	UNP Q96W94
D	461	HIS	-	EXPRESSION TAG	UNP Q96W94
D	462	HIS	-	EXPRESSION TAG	UNP Q96W94
D	463	HIS	-	EXPRESSION TAG	UNP Q96W94
E	456	HIS	-	EXPRESSION TAG	UNP Q96W94
E	457	HIS	-	EXPRESSION TAG	UNP Q96W94
E	458	HIS	-	EXPRESSION TAG	UNP Q96W94
E	459	HIS	-	EXPRESSION TAG	UNP Q96W94
E	460	HIS	-	EXPRESSION TAG	UNP Q96W94
E	461	HIS	-	EXPRESSION TAG	UNP Q96W94
E	462	HIS	-	EXPRESSION TAG	UNP Q96W94
E	463	HIS	-	EXPRESSION TAG	UNP Q96W94
F	456	HIS	-	EXPRESSION TAG	UNP Q96W94
F	457	HIS	-	EXPRESSION TAG	UNP Q96W94
F	458	HIS	-	EXPRESSION TAG	UNP Q96W94
F	459	HIS	-	EXPRESSION TAG	UNP Q96W94
F	460	HIS	-	EXPRESSION TAG	UNP Q96W94
F	461	HIS	-	EXPRESSION TAG	UNP Q96W94
F	462	HIS	-	EXPRESSION TAG	UNP Q96W94
F	463	HIS	-	EXPRESSION TAG	UNP Q96W94
G	456	HIS	-	EXPRESSION TAG	UNP Q96W94
G	457	HIS	-	EXPRESSION TAG	UNP Q96W94
G	458	HIS	-	EXPRESSION TAG	UNP Q96W94
G	459	HIS	-	EXPRESSION TAG	UNP Q96W94
G	460	HIS	-	EXPRESSION TAG	UNP Q96W94
G	461	HIS	-	EXPRESSION TAG	UNP Q96W94
G	462	HIS	-	EXPRESSION TAG	UNP Q96W94

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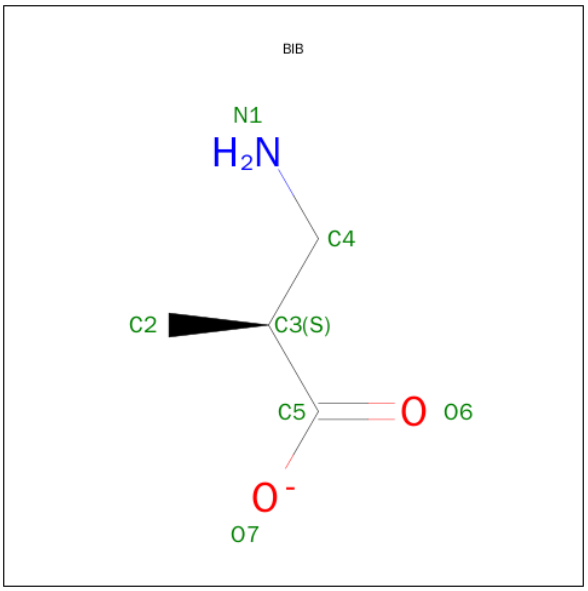
Chain	Residue	Modelled	Actual	Comment	Reference
G	463	HIS	-	EXPRESSION TAG	UNP Q96W94
H	456	HIS	-	EXPRESSION TAG	UNP Q96W94
H	457	HIS	-	EXPRESSION TAG	UNP Q96W94
H	458	HIS	-	EXPRESSION TAG	UNP Q96W94
H	459	HIS	-	EXPRESSION TAG	UNP Q96W94
H	460	HIS	-	EXPRESSION TAG	UNP Q96W94
H	461	HIS	-	EXPRESSION TAG	UNP Q96W94
H	462	HIS	-	EXPRESSION TAG	UNP Q96W94
H	463	HIS	-	EXPRESSION TAG	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: $C_4H_8NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 7 4 1 2	0	0
3	A	1	Total C N O 7 4 1 2	0	0
3	C	1	Total C N O 7 4 1 2	0	0
3	D	1	Total C N O 7 4 1 2	0	0
3	E	1	Total C N O 7 4 1 2	0	0
3	E	1	Total C N O 7 4 1 2	0	0
3	G	1	Total C N O 7 4 1 2	0	0
3	G	1	Total C N O 7 4 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	60	Total O 60 60	0	0
4	C	91	Total O 91 91	0	0
4	D	54	Total O 54 54	0	0

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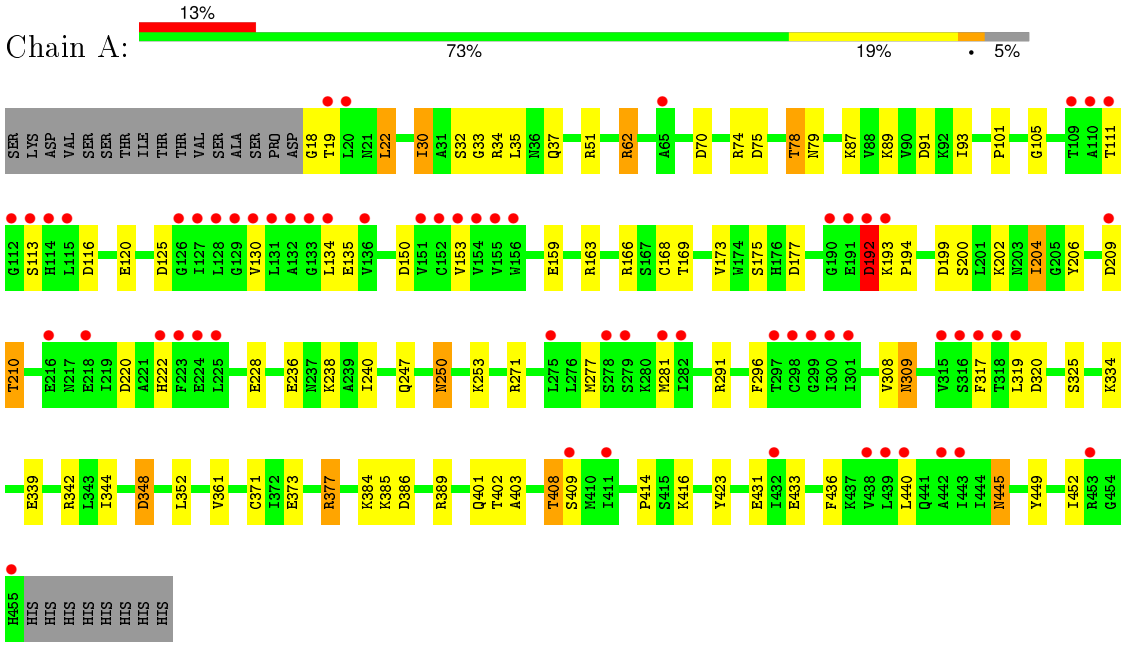
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	20	Total O 20 20	0	0
4	F	101	Total O 101 101	0	0
4	G	24	Total O 24 24	0	0
4	H	50	Total O 50 50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

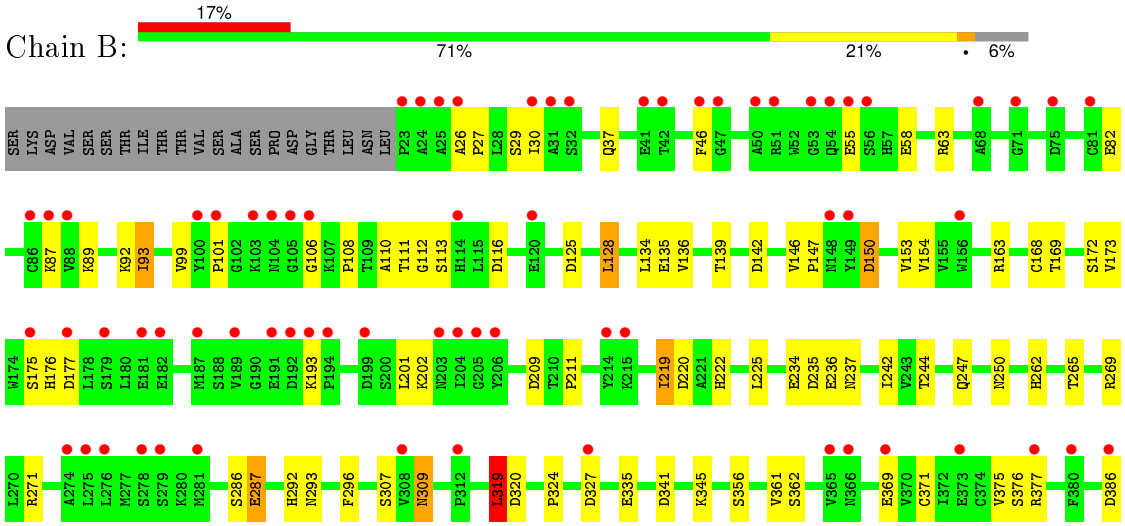
- Molecule 1: beta-alanine synthase

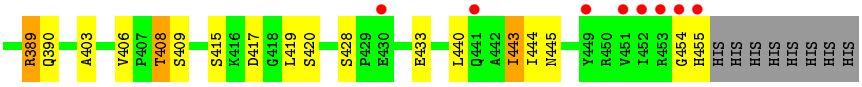
Chain A:



- Molecule 1: beta-alanine synthase

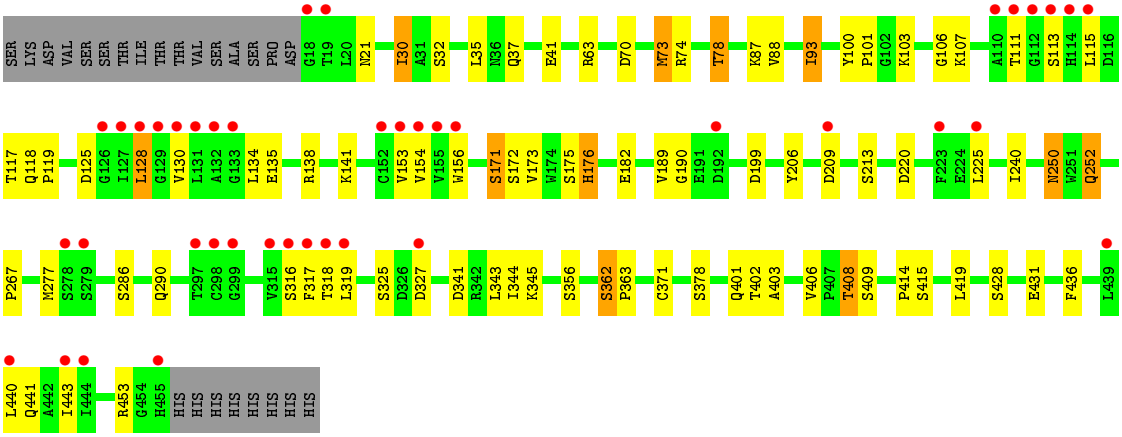
Chain B:





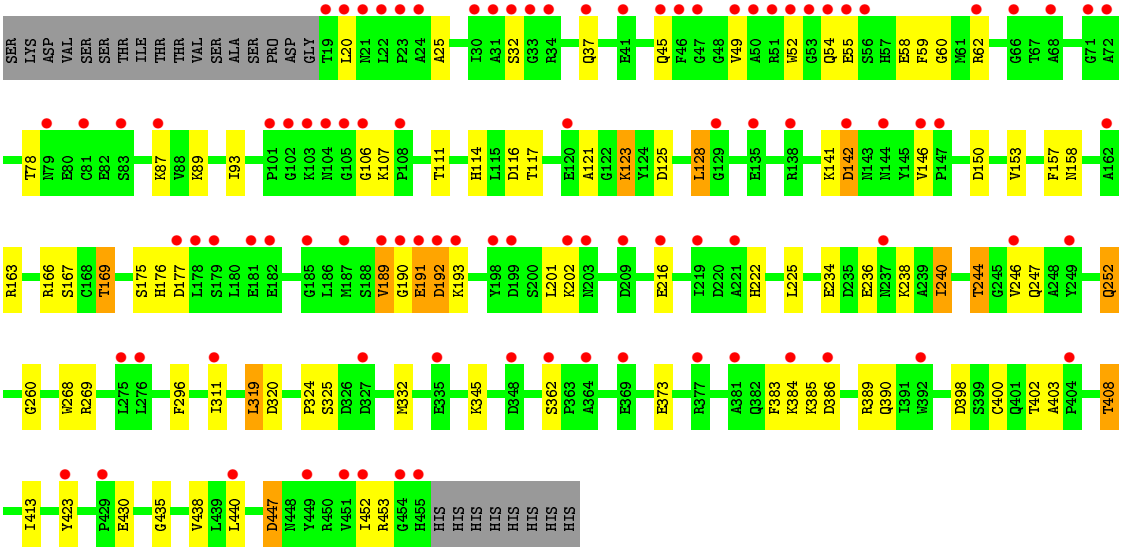
• Molecule 1: beta-alanine synthase

Chain C:



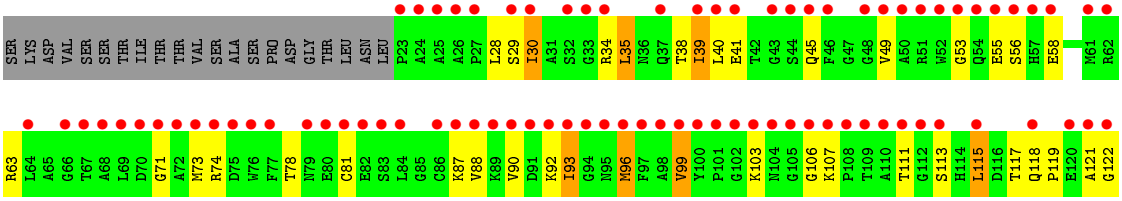
• Molecule 1: beta-alanine synthase

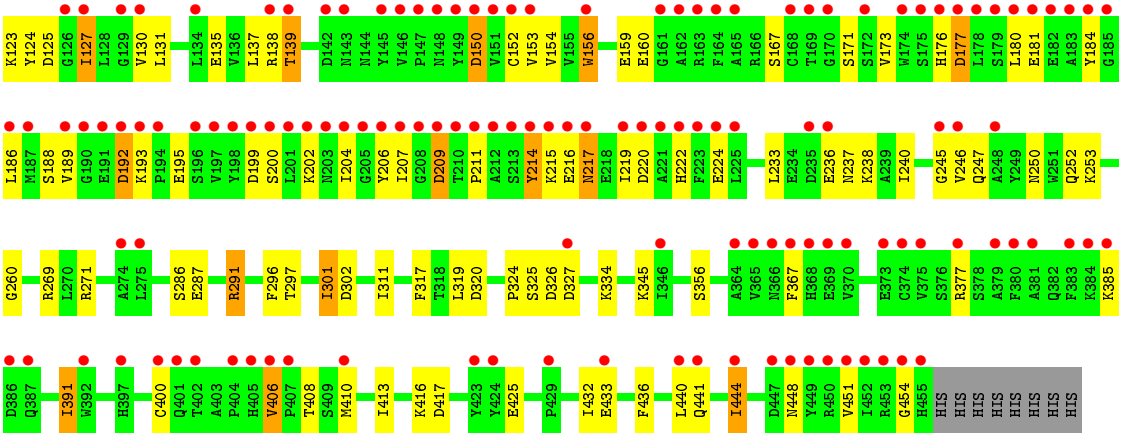
Chain D:



• Molecule 1: beta-alanine synthase

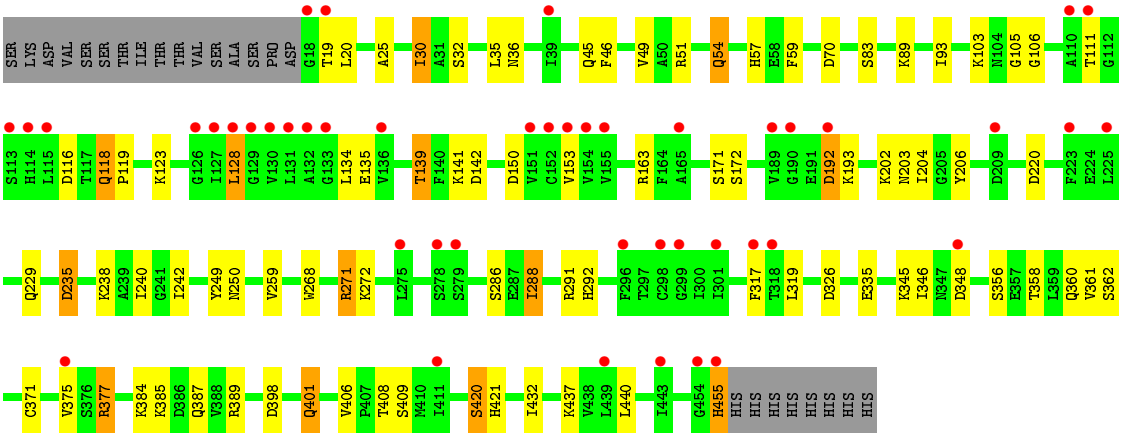
Chain E:





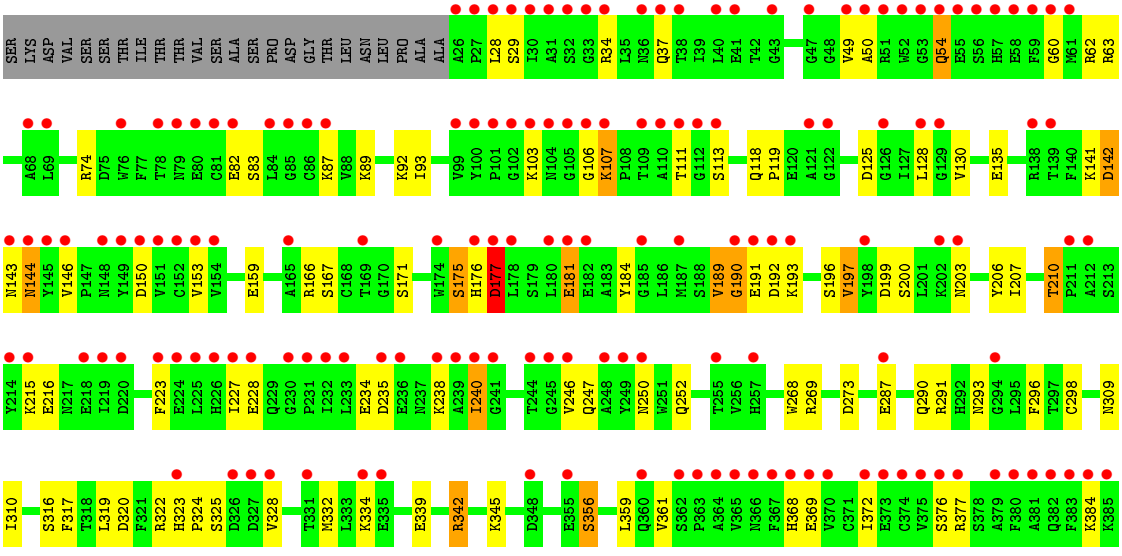
• Molecule 1: beta-alanine synthase

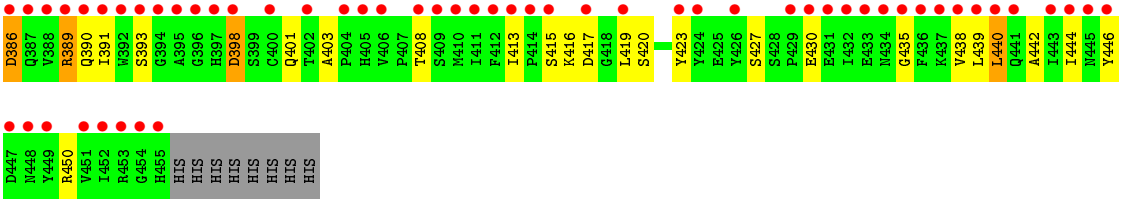
Chain F:



• Molecule 1: beta-alanine synthase

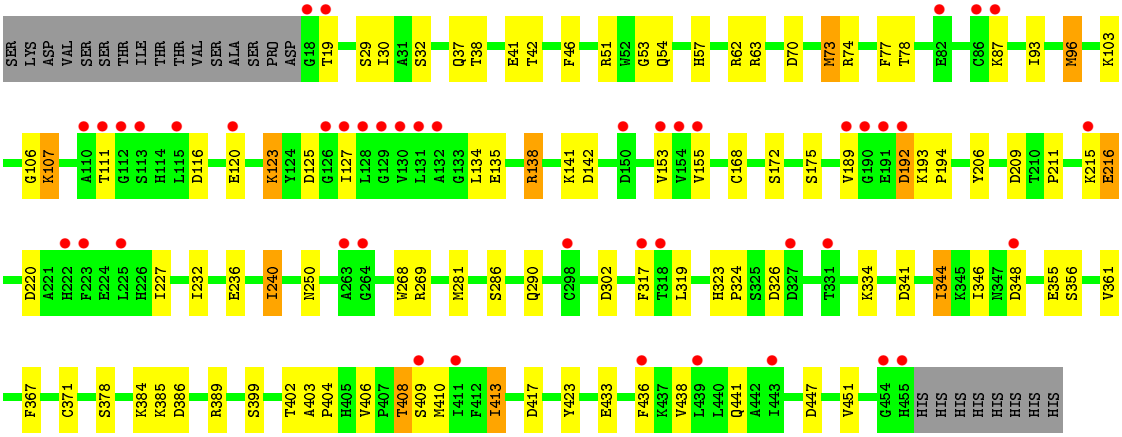
Chain G:





- Molecule 1: beta-alanine synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.23Å 77.12Å 225.52Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 24.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-2.70) 95.9 (24.90-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.266 0.299 , 0.333	Depositor DCC
R_{free} test set	5296 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	10 of 106175 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	27487	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.92 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5506e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BIB

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	0.56	1/3457 (0.0%)	0.80	15/4689 (0.3%)
1	B	0.43	0/3422	0.75	14/4640 (0.3%)
1	C	0.52	0/3457	0.75	6/4689 (0.1%)
1	D	0.44	0/3453	0.73	8/4684 (0.2%)
1	E	0.39	0/3422	0.71	10/4640 (0.2%)
1	F	0.49	0/3457	0.73	7/4689 (0.1%)
1	G	0.38	0/3404	0.72	13/4615 (0.3%)
1	H	0.44	0/3457	0.74	12/4689 (0.3%)
All	All	0.46	1/27529 (0.0%)	0.74	85/37335 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLY	C-O	-9.59	1.08	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	125	ASP	CB-CG-OD2	9.55	126.90	118.30
1	B	125	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	105	GLY	CA-C-N	8.52	133.25	116.20
1	D	125	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	309	ASN	CB-CA-C	-7.89	94.61	110.40
1	H	209	ASP	CB-CG-OD2	7.17	124.75	118.30
1	G	125	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	327	ASP	CB-CG-OD2	6.89	124.50	118.30
1	G	309	ASN	CB-CA-C	-6.83	96.73	110.40
1	B	142	ASP	CB-CG-OD2	6.76	124.39	118.30
1	C	125	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	319	LEU	CA-CB-CG	6.53	130.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	142	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	235	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	116	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	320	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	348	ASP	CB-CG-OD2	6.35	124.01	118.30
1	F	116	ASP	CB-CG-OD2	6.20	123.88	118.30
1	F	235	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	75	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	105	GLY	CA-C-O	-6.04	109.72	120.60
1	B	177	ASP	CB-CG-OD2	6.03	123.72	118.30
1	G	150	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	220	ASP	CB-CG-OD2	6.00	123.70	118.30
1	F	70	ASP	CB-CG-OD2	6.00	123.70	118.30
1	H	326	ASP	CB-CG-OD2	5.97	123.68	118.30
1	H	341	ASP	CB-CG-OD2	5.91	123.61	118.30
1	G	177	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	309	ASN	N-CA-CB	-5.86	100.05	110.60
1	H	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	150	ASP	CB-CG-OD2	5.77	123.49	118.30
1	G	273	ASP	CB-CG-OD2	5.75	123.48	118.30
1	E	302	ASP	CB-CG-OD2	5.74	123.47	118.30
1	G	440	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	320	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	192	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	220	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	386	ASP	CB-CG-OD2	5.63	123.37	118.30
1	F	142	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	302	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	209	ASP	CB-CG-OD2	5.58	123.32	118.30
1	F	326	ASP	CB-CG-OD2	5.55	123.30	118.30
1	G	386	ASP	CB-CG-OD2	5.53	123.27	118.30
1	H	386	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	447	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	199	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	220	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	70	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	70	ASP	CB-CG-OD2	5.47	123.23	118.30
1	F	220	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	320	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	192	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	220	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	116	ASP	CB-CG-OD2	5.35	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	142	ASP	CB-CG-OD2	5.35	123.12	118.30
1	G	320	ASP	CB-CG-OD2	5.34	123.11	118.30
1	G	417	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	447	ASP	CB-CG-OD2	5.32	123.09	118.30
1	G	192	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	150	ASP	CB-CG-OD2	5.32	123.08	118.30
1	E	326	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	105	GLY	N-CA-C	5.30	126.35	113.10
1	E	177	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	192	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	22	LEU	CA-CB-CG	5.26	127.40	115.30
1	E	320	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	348	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	327	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	125	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	209	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	199	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	220	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	199	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	341	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	417	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	327	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	150	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	177	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	70	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	209	ASP	CB-CG-OD2	5.06	122.85	118.30
1	G	235	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	398	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	150	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	199	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	341	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3379	0	3264	49	0
1	B	3344	0	3227	39	1
1	C	3379	0	3264	44	0
1	D	3375	0	3261	39	0
1	E	3344	0	3227	73	0
1	F	3379	0	3264	41	0
1	G	3327	0	3209	51	1
1	H	3379	0	3264	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	7	0	8	1	0
3	B	7	0	8	0	0
3	C	7	0	8	0	0
3	D	7	0	8	0	0
3	E	14	0	16	0	0
3	G	14	0	16	0	0
4	A	109	0	0	4	0
4	B	60	0	0	3	0
4	C	91	0	0	2	0
4	D	54	0	0	3	0
4	E	20	0	0	0	0
4	F	101	0	0	3	0
4	G	24	0	0	3	0
4	H	50	0	0	2	0
All	All	27487	0	26044	370	1

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

All (370) 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:D:189:VAL:HG23	1:D:190:GLY:H	1.24	1.03
1:E:118:GLN:HG3	1:E:119:PRO:HD2	1.47	0.96
1:E:71:GLY:HA3	1:E:204:ILE:CG2	1.97	0.94
1:H:346:ILE:HD11	4:H:511:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:HB2	1:B:58:GLU:HG3	1.49	0.90
1:E:78:THR:HG23	1:E:88:VAL:HG11	1.54	0.89
1:E:211:PRO:O	1:E:217:ASN:ND2	2.06	0.89
1:C:189:VAL:HG23	1:C:190:GLY:H	1.40	0.86
1:F:135:GLU:O	1:F:139:THR:HG23	1.78	0.82
1:E:247:GLN:HE21	1:E:324:PRO:HD3	1.46	0.81
1:C:118:GLN:HG3	1:C:119:PRO:HD2	1.63	0.81
1:E:135:GLU:O	1:E:139:THR:HG23	1.80	0.80
1:B:371:CYS:HB3	1:B:409:SER:HB3	1.63	0.79
1:F:118:GLN:HG3	1:F:119:PRO:CD	2.12	0.78
1:E:448:ASN:O	1:E:451:VAL:HG12	1.84	0.78
1:D:296:PHE:CE1	1:D:319:LEU:HD23	2.19	0.78
1:E:30:ILE:CG2	1:E:436:PHE:HE2	1.96	0.78
1:H:74:ARG:O	1:H:78:THR:HG23	1.84	0.77
1:E:71:GLY:HA3	1:E:204:ILE:HG21	1.64	0.77
1:A:309:ASN:HD21	3:A:2502:BIB:H3	1.50	0.77
1:B:112:GLY:HA3	1:B:154:VAL:HG22	1.65	0.76
1:C:37:GLN:O	1:C:41:GLU:HG3	1.86	0.75
1:E:71:GLY:CA	1:E:204:ILE:HG21	2.17	0.74
1:D:413:ILE:HD11	1:D:435:GLY:CA	2.19	0.73
1:E:71:GLY:HA3	1:E:204:ILE:HG23	1.69	0.72
1:C:74:ARG:O	1:C:78:THR:HG22	1.90	0.72
1:D:296:PHE:HE1	1:D:319:LEU:HD23	1.52	0.72
1:D:189:VAL:HG23	1:D:190:GLY:N	2.02	0.72
1:H:62:ARG:HD2	4:H:538:HOH:O	1.90	0.72
1:F:455:HIS:CD2	1:F:455:HIS:N	2.58	0.71
1:C:317:PHE:CE1	1:C:319:LEU:HD21	2.25	0.70
1:G:89:LYS:HB3	1:G:210:THR:HG21	1.74	0.70
1:E:236:GLU:O	1:E:238:LYS:HE3	1.91	0.70
1:C:118:GLN:HG3	1:C:119:PRO:CD	2.22	0.70
1:C:371:CYS:HB3	1:C:409:SER:HB2	1.74	0.69
1:E:53:GLY:HA3	1:E:58:GLU:OE1	1.92	0.69
1:A:74:ARG:O	1:A:78:THR:HG22	1.92	0.69
1:C:63:ARG:CZ	1:C:73:MET:HG3	2.23	0.69
1:E:96:MET:SD	1:E:206:TYR:HE2	2.16	0.68
1:F:118:GLN:HG3	1:F:119:PRO:HD2	1.74	0.68
1:H:317:PHE:CE1	1:H:319:LEU:HD21	2.28	0.68
1:D:247:GLN:HE21	1:D:324:PRO:HD3	1.58	0.68
1:D:189:VAL:CG2	1:D:190:GLY:H	2.06	0.67
1:A:371:CYS:HB3	1:A:409:SER:HB2	1.77	0.67
1:E:269:ARG:NH2	1:F:235:ASP:OD1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:OE2	4:A:2567:HOH:O	2.11	0.67
1:C:189:VAL:HG23	1:C:190:GLY:N	2.07	0.66
1:D:244:THR:O	4:D:4531:HOH:O	2.14	0.66
1:C:182:GLU:OE1	4:C:3559:HOH:O	2.12	0.66
1:D:55:GLU:HB2	1:D:58:GLU:HG3	1.76	0.66
1:B:112:GLY:HA3	1:B:154:VAL:CG2	2.24	0.65
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.31	0.65
1:G:118:GLN:HG3	1:G:119:PRO:HD2	1.79	0.65
1:E:209:ASP:HB3	1:G:356:SER:O	1.97	0.65
1:D:403:ALA:HA	1:D:408:THR:HG23	1.79	0.65
1:B:110:ALA:HB2	1:B:219:ILE:HG12	1.77	0.65
1:G:413:ILE:HD11	1:G:435:GLY:CA	2.27	0.65
1:E:28:LEU:HD11	1:E:444:ILE:HD11	1.78	0.64
1:E:71:GLY:CA	1:E:204:ILE:CG2	2.72	0.64
1:F:105:GLY:HA3	4:F:591:HOH:O	1.97	0.64
1:G:29:SER:HB3	1:G:143:ASN:HD21	1.63	0.64
1:E:181:GLU:HG2	1:G:334:LYS:HE2	1.80	0.64
1:F:57:HIS:O	1:F:123:LYS:HE2	1.97	0.63
1:G:403:ALA:HA	1:G:408:THR:HG22	1.80	0.63
1:F:406:VAL:O	1:F:408:THR:HG23	1.99	0.63
1:D:123:LYS:HD3	4:D:4510:HOH:O	1.99	0.62
1:F:36:ASN:HD22	1:F:432:ILE:HD12	1.64	0.62
1:A:339:GLU:OE2	1:A:342:ARG:NH1	2.31	0.62
1:E:88:VAL:O	1:E:88:VAL:HG13	1.99	0.62
1:A:30:ILE:HG12	1:A:436:PHE:HE2	1.65	0.61
1:F:317:PHE:CE1	1:F:319:LEU:HD21	2.35	0.61
1:G:413:ILE:HD11	1:G:435:GLY:HA3	1.82	0.61
1:B:99:VAL:HG21	4:B:1533:HOH:O	2.01	0.61
1:F:118:GLN:HG3	1:F:119:PRO:HD3	1.82	0.60
1:E:63:ARG:HH12	1:E:115:LEU:HB3	1.65	0.60
1:E:118:GLN:HG3	1:E:119:PRO:CD	2.24	0.60
1:E:30:ILE:HG21	1:E:436:PHE:HE2	1.66	0.60
1:C:128:LEU:HD13	1:C:225:LEU:HG	1.83	0.60
1:D:55:GLU:HB2	1:D:58:GLU:CG	2.32	0.60
1:F:59:PHE:O	1:F:123:LYS:HE3	2.01	0.59
1:A:317:PHE:HE1	1:A:319:LEU:HD21	1.67	0.59
1:G:184:TYR:O	1:G:196:SER:HB2	2.02	0.59
1:F:25:ALA:O	4:F:576:HOH:O	2.17	0.59
1:E:317:PHE:CE1	1:E:319:LEU:HD21	2.38	0.59
1:D:413:ILE:HD11	1:D:435:GLY:HA3	1.83	0.59
1:B:128:LEU:HD13	1:B:225:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ARG:HB3	1:E:206:TYR:CZ	2.38	0.58
1:H:120:GLU:HG2	1:H:423:TYR:CZ	2.39	0.58
1:H:367:PHE:CE2	1:H:410:MET:HG3	2.38	0.58
1:C:35:LEU:HB2	1:C:135:GLU:HG3	1.86	0.58
1:C:135:GLU:OE1	1:C:138:ARG:NH1	2.32	0.58
1:H:37:GLN:O	1:H:41:GLU:HG3	2.03	0.58
1:A:120:GLU:HG2	1:A:423:TYR:CZ	2.38	0.58
1:E:35:LEU:HD12	1:E:436:PHE:HB2	1.85	0.58
1:D:60:GLY:HA3	1:D:423:TYR:CD2	2.38	0.58
1:E:137:LEU:HD11	1:E:153:VAL:HG23	1.86	0.58
1:G:49:VAL:HG12	1:G:50:ALA:N	2.18	0.58
1:F:242:ILE:HD12	1:F:375:VAL:HG12	1.85	0.58
1:G:368:HIS:O	1:G:372:ILE:HG12	2.04	0.58
1:E:219:ILE:HD11	1:E:406:VAL:HG21	1.85	0.57
1:D:413:ILE:HD11	1:D:435:GLY:HA2	1.84	0.57
1:E:123:LYS:HE2	1:E:124:TYR:CE1	2.39	0.57
1:A:62:ARG:HD3	4:A:2609:HOH:O	2.04	0.57
1:C:277:MET:HE1	1:C:343:LEU:O	2.04	0.57
1:H:134:LEU:HG	1:H:138:ARG:HD2	1.85	0.57
1:G:159:GLU:OE1	4:G:8505:HOH:O	2.17	0.57
1:B:27:PRO:HG2	1:G:328:VAL:HG22	1.84	0.57
1:G:184:TYR:HA	1:G:197:VAL:HG22	1.86	0.56
1:D:158:ASN:HB3	1:D:169:THR:HG23	1.86	0.56
1:A:308:VAL:HG23	4:A:2542:HOH:O	2.05	0.56
1:F:229:GLN:HG2	1:F:420:SER:OG	2.06	0.56
1:E:39:ILE:HG22	1:E:131:LEU:HD12	1.87	0.56
1:D:128:LEU:HD13	1:D:225:LEU:HG	1.89	0.55
1:F:135:GLU:O	1:F:139:THR:CG2	2.54	0.55
1:H:19:THR:O	1:H:19:THR:HG23	2.07	0.55
1:F:238:LYS:HD2	1:F:389:ARG:HB2	1.88	0.55
1:E:296:PHE:HE1	1:E:319:LEU:HD22	1.71	0.55
1:D:59:PHE:O	1:D:123:LYS:HD2	2.07	0.55
1:E:291:ARG:HH11	1:E:291:ARG:HB2	1.72	0.54
1:G:49:VAL:HG12	1:G:50:ALA:H	1.72	0.54
1:H:211:PRO:HG2	1:H:216:GLU:HG2	1.88	0.54
1:E:296:PHE:CE1	1:E:319:LEU:HD22	2.42	0.54
1:C:250:ASN:HD21	1:C:252:GLN:HE21	1.55	0.54
1:H:63:ARG:CZ	1:H:73:MET:HG3	2.38	0.54
1:B:175:SER:O	1:B:176:HIS:HB2	2.07	0.54
1:A:414:PRO:HD2	1:A:431:GLU:HG2	1.90	0.54
1:E:96:MET:SD	1:E:206:TYR:CE2	3.01	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ILE:HD12	1:E:317:PHE:HB3	1.90	0.53
1:A:101:PRO:HA	1:A:150:ASP:OD1	2.08	0.53
1:C:371:CYS:HB3	1:C:409:SER:CB	2.38	0.53
1:A:135:GLU:HG2	4:A:2564:HOH:O	2.07	0.53
1:F:455:HIS:N	1:F:455:HIS:HD2	2.04	0.53
1:B:371:CYS:HB3	1:B:409:SER:CB	2.36	0.53
1:E:93:ILE:HG13	1:E:173:VAL:HG21	1.91	0.53
1:E:123:LYS:HE2	1:E:124:TYR:HE1	1.74	0.53
1:A:204:ILE:HD12	1:A:206:TYR:CD1	2.44	0.53
1:D:222:HIS:HB3	1:D:408:THR:HB	1.91	0.52
1:G:240:ILE:HG12	1:G:438:VAL:HG21	1.91	0.52
1:H:371:CYS:CB	1:H:409:SER:HB2	2.40	0.52
1:G:247:GLN:HE21	1:G:324:PRO:HD3	1.74	0.52
1:E:233:LEU:HD22	1:E:238:LYS:HB2	1.91	0.52
1:F:35:LEU:HB2	1:F:135:GLU:HG3	1.92	0.52
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.74	0.52
1:G:317:PHE:HE1	1:G:319:LEU:HD21	1.74	0.52
1:B:101:PRO:HA	1:B:150:ASP:OD1	2.10	0.52
1:B:247:GLN:HE21	1:B:324:PRO:HD3	1.75	0.52
1:E:34:ARG:HD3	1:E:135:GLU:OE1	2.10	0.52
1:A:30:ILE:HD11	1:A:440:LEU:CD2	2.40	0.52
1:F:371:CYS:HB3	1:F:409:SER:HB2	1.92	0.52
1:E:211:PRO:O	1:E:217:ASN:CG	2.49	0.51
1:E:222:HIS:HB3	1:E:408:THR:HG22	1.92	0.51
1:G:175:SER:OG	1:G:401:GLN:O	2.27	0.51
1:A:403:ALA:HA	1:A:408:THR:HG23	1.93	0.51
1:E:291:ARG:HH11	1:E:291:ARG:CB	2.23	0.51
1:F:292:HIS:HE1	1:F:335:GLU:OE1	1.93	0.51
1:B:296:PHE:HE1	1:B:319:LEU:HB3	1.74	0.51
1:C:37:GLN:O	1:C:41:GLU:CG	2.58	0.51
1:F:54:GLN:HG2	4:F:555:HOH:O	2.10	0.51
1:A:204:ILE:HD12	1:A:206:TYR:HD1	1.75	0.51
1:H:135:GLU:HB3	1:H:436:PHE:CE1	2.46	0.51
1:E:137:LEU:HD11	1:E:153:VAL:CG2	2.41	0.51
1:H:227:ILE:HA	1:H:413:ILE:HD13	1.92	0.51
1:G:74:ARG:HB3	1:G:206:TYR:CZ	2.46	0.51
1:F:317:PHE:HE1	1:F:319:LEU:HD21	1.74	0.50
1:H:51:ARG:NH1	1:H:53:GLY:O	2.41	0.50
1:D:240:ILE:HG12	1:D:438:VAL:HG21	1.92	0.50
1:D:114:HIS:HB2	1:D:116:ASP:OD1	2.11	0.50
1:G:166:ARG:HG3	1:G:166:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:413:ILE:HD11	1:G:435:GLY:HA2	1.92	0.50
1:A:449:TYR:HA	1:A:452:ILE:HD12	1.93	0.50
1:C:93:ILE:HG13	1:C:173:VAL:HG21	1.93	0.50
1:F:20:LEU:O	1:F:377:ARG:NH1	2.43	0.50
1:D:166:ARG:O	1:D:169:THR:HG22	2.10	0.50
1:G:171:SER:O	1:G:175:SER:HB2	2.11	0.50
1:D:238:LYS:HD2	1:D:389:ARG:HB2	1.92	0.50
1:D:175:SER:O	1:D:176:HIS:HB2	2.12	0.50
1:E:30:ILE:HG22	1:E:436:PHE:HE2	1.75	0.50
1:A:204:ILE:HD12	1:A:206:TYR:HB2	1.93	0.50
1:G:446:TYR:CE2	1:G:450:ARG:HD2	2.47	0.50
1:H:346:ILE:HD13	1:H:346:ILE:N	2.27	0.49
1:H:403:ALA:N	1:H:404:PRO:CD	2.75	0.49
1:A:371:CYS:HB3	1:A:409:SER:CB	2.42	0.49
1:C:267:PRO:HB2	4:C:3548:HOH:O	2.11	0.49
1:B:92:LYS:HD2	1:B:211:PRO:HA	1.94	0.49
1:E:88:VAL:O	1:E:88:VAL:CG1	2.61	0.49
1:F:111:THR:O	1:F:153:VAL:HA	2.12	0.49
1:G:238:LYS:HD2	1:G:389:ARG:HB2	1.94	0.49
1:A:236:GLU:OE2	1:B:269:ARG:NH2	2.45	0.49
1:C:172:SER:HA	1:C:401:GLN:HE21	1.78	0.49
1:G:403:ALA:HA	1:G:408:THR:CG2	2.43	0.49
1:H:371:CYS:HB3	1:H:409:SER:HB2	1.95	0.49
1:B:169:THR:O	1:B:173:VAL:HG13	2.11	0.49
1:B:26:ALA:HB2	1:G:291:ARG:O	2.13	0.49
1:E:34:ARG:CZ	1:E:138:ARG:HD2	2.42	0.49
1:C:378:SER:OG	1:C:441:GLN:HB3	2.11	0.49
1:E:233:LEU:HD21	1:E:391:ILE:HD11	1.94	0.48
1:A:222:HIS:O	1:A:408:THR:HB	2.13	0.48
1:E:214:TYR:H	1:E:214:TYR:HD1	1.61	0.48
1:A:371:CYS:CB	1:A:409:SER:HB2	2.43	0.48
1:E:211:PRO:O	1:E:217:ASN:OD1	2.31	0.48
1:C:371:CYS:CB	1:C:409:SER:HB2	2.43	0.48
1:D:269:ARG:HH11	1:D:269:ARG:HG2	1.77	0.48
1:H:406:VAL:HG23	1:H:408:THR:HG22	1.96	0.48
1:G:317:PHE:CE1	1:G:319:LEU:HD21	2.49	0.48
1:H:227:ILE:HG22	1:H:413:ILE:HD11	1.96	0.48
1:A:192:ASP:O	1:A:194:PRO:HD3	2.14	0.48
1:G:111:THR:O	1:G:153:VAL:HA	2.14	0.47
1:F:249:TYR:CE2	1:F:362:SER:HB3	2.49	0.47
1:A:159:GLU:HG2	1:A:168:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD21	1:E:130:VAL:HG21	1.96	0.47
1:A:34:ARG:HG2	1:A:135:GLU:OE1	2.13	0.47
1:H:57:HIS:O	1:H:123:LYS:HE2	2.15	0.47
1:A:402:THR:OG1	1:A:408:THR:HG21	2.15	0.47
1:E:122:GLY:HA3	1:E:425:GLU:HB3	1.96	0.47
1:A:33:GLY:O	1:A:37:GLN:HG2	2.14	0.47
1:H:240:ILE:HG12	1:H:438:VAL:HG21	1.96	0.47
1:B:287:GLU:HG3	4:B:1549:HOH:O	2.15	0.47
1:D:403:ALA:HA	1:D:408:THR:CG2	2.45	0.47
1:B:440:LEU:O	1:B:444:ILE:HG13	2.15	0.47
1:E:317:PHE:HE1	1:E:319:LEU:HD21	1.77	0.46
1:H:402:THR:OG1	1:H:408:THR:HG21	2.16	0.46
1:F:249:TYR:OH	1:F:360:GLN:NE2	2.47	0.46
1:A:250:ASN:HD22	1:A:250:ASN:C	2.18	0.46
1:G:60:GLY:HA3	1:G:423:TYR:CD2	2.50	0.46
1:E:78:THR:CG2	1:E:88:VAL:HG11	2.35	0.46
1:E:30:ILE:HG21	1:E:436:PHE:CE2	2.49	0.46
1:A:18:GLY:HA2	1:A:22:LEU:HD13	1.96	0.46
1:H:111:THR:O	1:H:153:VAL:HA	2.14	0.46
1:A:339:GLU:CD	1:A:342:ARG:NH1	2.69	0.46
1:H:46:PHE:CD1	1:H:73:MET:HG2	2.50	0.46
1:A:277:MET:HG3	1:A:352:LEU:HD22	1.96	0.46
1:E:246:VAL:HG21	1:E:400:CYS:SG	2.55	0.46
1:G:113:SER:HB3	1:G:130:VAL:HG23	1.98	0.46
1:C:403:ALA:HA	1:C:408:THR:HG23	1.96	0.46
1:H:232:ILE:O	1:H:236:GLU:HG3	2.16	0.46
1:F:259:VAL:HG23	1:F:272:LYS:HD2	1.98	0.46
1:B:406:VAL:HG23	1:B:408:THR:HG22	1.97	0.46
1:E:74:ARG:HB3	1:E:206:TYR:OH	2.16	0.45
1:C:406:VAL:HG23	1:C:408:THR:HG22	1.97	0.45
1:B:111:THR:O	1:B:153:VAL:HA	2.17	0.45
1:C:100:TYR:HA	1:C:101:PRO:HD3	1.81	0.45
1:B:234:GLU:OE2	1:B:417:ASP:N	2.46	0.45
1:E:38:THR:HG21	1:E:138:ARG:HH22	1.81	0.45
1:C:74:ARG:HB3	1:C:206:TYR:CZ	2.51	0.45
1:E:111:THR:O	1:E:153:VAL:HA	2.16	0.45
1:B:236:GLU:OE1	1:B:389:ARG:HD2	2.16	0.45
1:F:36:ASN:ND2	1:F:432:ILE:HD12	2.31	0.45
1:H:168:CYS:O	1:H:172:SER:OG	2.32	0.45
1:A:281:MET:HE3	1:A:344:ILE:HD13	1.98	0.45
1:C:171:SER:O	1:C:175:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:HIS:HE1	1:B:335:GLU:OE1	2.00	0.45
1:B:136:VAL:HG21	1:B:443:ILE:HD11	1.99	0.45
1:H:96:MET:HG3	1:H:155:VAL:HB	1.99	0.45
1:A:35:LEU:HB2	1:A:135:GLU:HG3	1.99	0.45
1:E:297:THR:OG1	1:F:271:ARG:NH2	2.49	0.45
1:F:118:GLN:HE22	1:F:421:HIS:CE1	2.34	0.45
1:G:111:THR:HG23	1:G:439:LEU:HD11	1.98	0.45
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.76	0.45
1:B:55:GLU:HB2	1:B:58:GLU:CG	2.34	0.45
1:F:118:GLN:NE2	1:F:421:HIS:CE1	2.85	0.45
1:F:204:ILE:HD12	1:F:206:TYR:CD1	2.51	0.45
1:C:30:ILE:HD11	1:C:440:LEU:HD22	1.99	0.44
1:G:246:VAL:HG22	1:G:393:SER:HB3	1.98	0.44
1:A:445:ASN:HD22	1:A:445:ASN:HA	1.64	0.44
1:H:30:ILE:HG13	1:H:30:ILE:O	2.17	0.44
1:D:246:VAL:HG21	1:D:400:CYS:SG	2.57	0.44
1:C:154:VAL:HG11	1:C:156:TRP:CE2	2.53	0.44
1:C:176:HIS:HE1	1:C:213:SER:OG	2.00	0.44
1:F:128:LEU:HD21	1:F:432:ILE:HG23	1.99	0.44
1:F:45:GLN:HG2	1:F:46:PHE:CE1	2.52	0.44
1:D:157:PHE:CE1	1:D:201:LEU:HD21	2.52	0.44
1:G:268:TRP:CE2	1:H:290:GLN:HG2	2.53	0.44
1:A:277:MET:CG	1:A:352:LEU:HD22	2.47	0.44
1:H:323:HIS:CG	1:H:324:PRO:HD2	2.52	0.44
1:G:310:ILE:HD12	4:G:8520:HOH:O	2.18	0.44
1:E:245:GLY:HA2	1:E:367:PHE:CD1	2.53	0.44
1:D:163:ARG:NH1	1:D:191:GLU:OE1	2.51	0.44
1:C:30:ILE:HG12	1:C:436:PHE:HE2	1.82	0.43
1:G:176:HIS:HA	4:G:8523:HOH:O	2.17	0.43
1:H:317:PHE:HE1	1:H:319:LEU:HD21	1.80	0.43
1:H:281:MET:CE	1:H:344:ILE:HG23	2.48	0.43
1:G:323:HIS:ND1	1:G:324:PRO:HD2	2.33	0.43
1:H:107:LYS:HG3	1:H:107:LYS:H	1.55	0.43
1:D:111:THR:O	1:D:153:VAL:HA	2.19	0.43
1:C:73:MET:CE	1:C:115:LEU:HD22	2.49	0.43
1:H:120:GLU:HG2	1:H:423:TYR:CE2	2.54	0.43
1:E:99:VAL:HG12	1:E:99:VAL:O	2.18	0.43
1:B:93:ILE:HG23	1:B:93:ILE:O	2.19	0.43
1:F:371:CYS:CB	1:F:409:SER:HB2	2.47	0.43
1:G:189:VAL:HG12	1:G:190:GLY:H	1.83	0.43
1:A:113:SER:HB3	1:A:130:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:SER:HB3	1:C:130:VAL:HG23	1.99	0.43
1:A:169:THR:O	1:A:173:VAL:HG23	2.19	0.43
1:G:107:LYS:O	1:G:450:ARG:NH2	2.50	0.43
1:C:406:VAL:O	1:C:408:THR:HG23	2.19	0.43
1:B:222:HIS:O	1:B:408:THR:HB	2.19	0.43
1:E:117:THR:HB	1:E:121:ALA:CB	2.49	0.43
1:A:177:ASP:OD2	1:A:401:GLN:NE2	2.52	0.43
1:D:52:TRP:CZ2	1:D:58:GLU:HA	2.54	0.43
1:E:291:ARG:HH11	1:E:291:ARG:CG	2.32	0.43
1:B:108:PRO:HG2	1:B:219:ILE:HG13	2.01	0.43
1:E:156:TRP:HZ3	1:E:222:HIS:NE2	2.16	0.43
1:A:89:LYS:CD	1:A:210:THR:HG21	2.49	0.43
1:G:247:GLN:NE2	1:G:324:PRO:HD3	2.33	0.42
1:B:445:ASN:HD22	1:B:445:ASN:HA	1.69	0.42
1:D:117:THR:HB	1:D:121:ALA:CB	2.48	0.42
1:A:236:GLU:OE2	1:A:389:ARG:NH1	2.52	0.42
1:A:91:ASP:HB2	1:A:210:THR:O	2.20	0.42
1:C:344:ILE:HG23	1:C:345:LYS:HD3	1.99	0.42
1:E:124:TYR:CD2	1:E:432:ILE:HD11	2.55	0.42
1:H:371:CYS:HB2	1:H:409:SER:HB2	2.02	0.42
1:B:168:CYS:O	1:B:172:SER:HB2	2.20	0.42
1:E:271:ARG:CZ	1:E:311:ILE:HD11	2.50	0.42
1:D:252:GLN:HB2	4:D:4554:HOH:O	2.20	0.42
1:A:296:PHE:CE1	1:A:319:LEU:HD22	2.54	0.42
1:B:262:HIS:HB3	1:B:265:THR:OG1	2.19	0.42
1:C:63:ARG:HB3	1:C:117:THR:HG23	2.01	0.42
1:A:30:ILE:HD11	1:A:440:LEU:HD22	2.01	0.42
1:F:171:SER:OG	1:F:398:ASP:OD1	2.37	0.42
1:C:318:THR:C	1:C:319:LEU:HD23	2.40	0.42
1:F:288:ILE:HG13	1:F:291:ARG:NH2	2.34	0.42
1:C:362:SER:HA	1:C:363:PRO:HD3	1.79	0.42
1:C:414:PRO:HG2	1:C:431:GLU:CD	2.39	0.42
1:H:378:SER:OG	1:H:441:GLN:HB3	2.19	0.42
1:F:172:SER:HA	1:F:401:GLN:HG3	2.02	0.42
1:E:93:ILE:O	1:E:93:ILE:HG23	2.20	0.42
1:C:111:THR:O	1:C:153:VAL:HA	2.19	0.42
1:G:175:SER:HB3	1:G:177:ASP:OD2	2.19	0.42
1:G:49:VAL:CG1	1:G:50:ALA:N	2.83	0.41
1:G:296:PHE:HE1	1:G:319:LEU:HD22	1.85	0.41
1:D:189:VAL:CG2	1:D:190:GLY:N	2.73	0.41
1:G:298:CYS:SG	1:G:317:PHE:HB2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:THR:OG1	1:C:408:THR:HG21	2.20	0.41
1:B:403:ALA:HA	1:B:408:THR:HG23	2.02	0.41
1:F:268:TRP:HA	1:F:271:ARG:HD3	2.02	0.41
1:G:290:GLN:HG3	1:H:268:TRP:CE2	2.55	0.41
1:E:127:ILE:H	1:E:127:ILE:HG12	1.53	0.41
1:C:290:GLN:HG2	1:D:268:TRP:CE2	2.55	0.41
1:H:74:ARG:HB3	1:H:206:TYR:CZ	2.56	0.41
1:D:402:THR:OG1	1:D:408:THR:HG21	2.20	0.41
1:H:127:ILE:H	1:H:127:ILE:HG12	1.62	0.41
1:G:398:ASP:N	1:G:398:ASP:OD1	2.44	0.41
1:G:339:GLU:OE2	1:G:342:ARG:NH1	2.52	0.41
1:C:78:THR:HB	1:C:88:VAL:HG11	2.01	0.41
1:B:319:LEU:N	1:B:319:LEU:HD23	2.36	0.41
1:A:22:LEU:HD11	1:A:449:TYR:HB2	2.02	0.41
1:B:242:ILE:HD12	1:B:375:VAL:HG12	2.02	0.41
1:A:111:THR:O	1:A:153:VAL:HA	2.21	0.41
1:B:443:ILE:H	1:B:443:ILE:HG12	1.71	0.41
1:H:192:ASP:O	1:H:194:PRO:HD3	2.21	0.41
1:G:181:GLU:H	1:G:181:GLU:HG3	1.57	0.41
1:E:38:THR:HG21	1:E:138:ARG:NH2	2.36	0.41
1:E:260:GLY:HA2	1:E:311:ILE:O	2.21	0.41
1:F:30:ILE:HD11	1:F:440:LEU:CD2	2.50	0.41
1:G:223:PHE:CE2	1:G:442:ALA:HB1	2.56	0.41
1:E:224:GLU:HB3	1:E:410:MET:HG2	2.03	0.41
1:G:54:GLN:HE21	1:G:54:GLN:HB3	1.70	0.41
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.90	0.41
1:D:240:ILE:HD13	1:D:383:PHE:CE1	2.56	0.41
1:G:413:ILE:CD1	1:G:435:GLY:HA3	2.50	0.40
1:H:87:LYS:HB2	1:H:87:LYS:NZ	2.36	0.40
1:D:166:ARG:NH1	1:D:167:SER:O	2.55	0.40
1:D:260:GLY:HA2	1:D:311:ILE:O	2.22	0.40
1:H:38:THR:O	1:H:42:THR:HG23	2.21	0.40
1:E:38:THR:HA	1:E:41:GLU:HG2	2.02	0.40
1:H:77:PHE:CD2	1:H:96:MET:CE	3.04	0.40
1:E:125:ASP:O	1:E:127:ILE:HG12	2.22	0.40
1:B:361:VAL:N	4:B:1525:HOH:O	2.49	0.40
1:B:46:PHE:O	1:B:63:ARG:HD3	2.21	0.40
1:A:238:LYS:HD3	1:A:386:ASP:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

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	436/462 (94%)	420 (96%)	16 (4%)	0	100	100
1	B	431/462 (93%)	418 (97%)	11 (3%)	2 (0%)	34	63
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	34	63
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	21	49
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	34	63
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	34	63
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	21	49
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	52	80
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	34	63

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	B	106	GLY
1	B	454	GLY
1	C	21	ASN
1	C	106	GLY
1	D	25	ALA
1	E	106	GLY
1	F	106	GLY
1	G	106	GLY
1	G	189	VAL
1	G	190	GLY
1	H	106	GLY

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Mol	Chain	Res	Type
1	D	106	GLY
1	F	192	ASP
1	G	191	GLU
1	E	454	GLY
1	D	189	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	360/383 (94%)	323 (90%)	37 (10%)	9 20
1	B	356/383 (93%)	314 (88%)	42 (12%)	6 15
1	C	360/383 (94%)	332 (92%)	28 (8%)	16 35
1	D	360/383 (94%)	317 (88%)	43 (12%)	6 15
1	E	356/383 (93%)	284 (80%)	72 (20%)	1 4
1	F	360/383 (94%)	321 (89%)	39 (11%)	8 18
1	G	355/383 (93%)	289 (81%)	66 (19%)	2 5
1	H	360/383 (94%)	325 (90%)	35 (10%)	10 23
All	All	2867/3064 (94%)	2505 (87%)	362 (13%)	5 13

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	30	ILE
1	A	32	SER
1	A	51	ARG
1	A	62	ARG
1	A	78	THR
1	A	79	ASN
1	A	87	LYS
1	A	93	ILE
1	A	134	LEU

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Mol	Chain	Res	Type
1	A	163	ARG
1	A	166	ARG
1	A	175	SER
1	A	192	ASP
1	A	193	LYS
1	A	200	SER
1	A	202	LYS
1	A	204	ILE
1	A	210	THR
1	A	240	ILE
1	A	247	GLN
1	A	250	ASN
1	A	253	LYS
1	A	271	ARG
1	A	291	ARG
1	A	325	SER
1	A	334	LYS
1	A	348	ASP
1	A	361	VAL
1	A	373	GLU
1	A	377	ARG
1	A	384	LYS
1	A	385	LYS
1	A	408	THR
1	A	416	LYS
1	A	433	GLU
1	A	445	ASN
1	B	29	SER
1	B	30	ILE
1	B	37	GLN
1	B	82	GLU
1	B	87	LYS
1	B	89	LYS
1	B	93	ILE
1	B	113	SER
1	B	128	LEU
1	B	134	LEU
1	B	135	GLU
1	B	139	THR
1	B	163	ARG
1	B	193	LYS
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	202	LYS
1	B	219	ILE
1	B	237	ASN
1	B	244	THR
1	B	250	ASN
1	B	271	ARG
1	B	286	SER
1	B	287	GLU
1	B	307	SER
1	B	309	ASN
1	B	319	LEU
1	B	345	LYS
1	B	356	SER
1	B	362	SER
1	B	369	GLU
1	B	376	SER
1	B	377	ARG
1	B	389	ARG
1	B	390	GLN
1	B	408	THR
1	B	415	SER
1	B	419	LEU
1	B	420	SER
1	B	428	SER
1	B	433	GLU
1	B	443	ILE
1	B	455	HIS
1	C	30	ILE
1	C	32	SER
1	C	73	MET
1	C	78	THR
1	C	87	LYS
1	C	93	ILE
1	C	103	LYS
1	C	107	LYS
1	C	128	LEU
1	C	134	LEU
1	C	141	LYS
1	C	171	SER
1	C	176	HIS
1	C	209	ASP
1	C	240	ILE

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	252	GLN
1	C	286	SER
1	C	316	SER
1	C	325	SER
1	C	356	SER
1	C	362	SER
1	C	408	THR
1	C	415	SER
1	C	419	LEU
1	C	428	SER
1	C	443	ILE
1	C	453	ARG
1	D	32	SER
1	D	37	GLN
1	D	45	GLN
1	D	49	VAL
1	D	54	GLN
1	D	62	ARG
1	D	78	THR
1	D	87	LYS
1	D	89	LYS
1	D	93	ILE
1	D	107	LYS
1	D	123	LYS
1	D	128	LEU
1	D	141	LYS
1	D	142	ASP
1	D	146	VAL
1	D	169	THR
1	D	191	GLU
1	D	192	ASP
1	D	193	LYS
1	D	202	LYS
1	D	216	GLU
1	D	234	GLU
1	D	236	GLU
1	D	240	ILE
1	D	244	THR
1	D	252	GLN
1	D	319	LEU
1	D	325	SER

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Mol	Chain	Res	Type
1	D	332	MET
1	D	345	LYS
1	D	362	SER
1	D	373	GLU
1	D	384	LYS
1	D	385	LYS
1	D	386	ASP
1	D	390	GLN
1	D	408	THR
1	D	430	GLU
1	D	440	LEU
1	D	447	ASP
1	D	452	ILE
1	D	453	ARG
1	E	29	SER
1	E	30	ILE
1	E	35	LEU
1	E	39	ILE
1	E	40	LEU
1	E	45	GLN
1	E	49	VAL
1	E	55	GLU
1	E	56	SER
1	E	73	MET
1	E	81	CYS
1	E	87	LYS
1	E	90	VAL
1	E	92	LYS
1	E	93	ILE
1	E	96	MET
1	E	99	VAL
1	E	103	LYS
1	E	107	LYS
1	E	113	SER
1	E	115	LEU
1	E	127	ILE
1	E	139	THR
1	E	150	ASP
1	E	152	CYS
1	E	154	VAL
1	E	156	TRP
1	E	159	GLU

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Mol	Chain	Res	Type
1	E	160	GLU
1	E	167	SER
1	E	171	SER
1	E	176	HIS
1	E	177	ASP
1	E	180	LEU
1	E	184	TYR
1	E	186	LEU
1	E	188	SER
1	E	189	VAL
1	E	192	ASP
1	E	193	LYS
1	E	195	GLU
1	E	200	SER
1	E	202	LYS
1	E	207	ILE
1	E	214	TYR
1	E	215	LYS
1	E	216	GLU
1	E	217	ASN
1	E	237	ASN
1	E	240	ILE
1	E	250	ASN
1	E	252	GLN
1	E	253	LYS
1	E	286	SER
1	E	287	GLU
1	E	291	ARG
1	E	301	ILE
1	E	325	SER
1	E	334	LYS
1	E	345	LYS
1	E	356	SER
1	E	377	ARG
1	E	385	LYS
1	E	391	ILE
1	E	406	VAL
1	E	413	ILE
1	E	416	LYS
1	E	417	ASP
1	E	433	GLU
1	E	440	LEU

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Mol	Chain	Res	Type
1	E	441	GLN
1	E	444	ILE
1	F	19	THR
1	F	30	ILE
1	F	32	SER
1	F	49	VAL
1	F	51	ARG
1	F	54	GLN
1	F	83	SER
1	F	89	LYS
1	F	93	ILE
1	F	103	LYS
1	F	118	GLN
1	F	128	LEU
1	F	134	LEU
1	F	139	THR
1	F	141	LYS
1	F	163	ARG
1	F	192	ASP
1	F	193	LYS
1	F	202	LYS
1	F	203	ASN
1	F	240	ILE
1	F	250	ASN
1	F	271	ARG
1	F	286	SER
1	F	288	ILE
1	F	345	LYS
1	F	346	ILE
1	F	348	ASP
1	F	356	SER
1	F	358	THR
1	F	361	VAL
1	F	377	ARG
1	F	384	LYS
1	F	385	LYS
1	F	387	GLN
1	F	401	GLN
1	F	420	SER
1	F	437	LYS
1	F	455	HIS
1	G	28	LEU

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Mol	Chain	Res	Type
1	G	34	ARG
1	G	37	GLN
1	G	54	GLN
1	G	62	ARG
1	G	63	ARG
1	G	82	GLU
1	G	83	SER
1	G	87	LYS
1	G	92	LYS
1	G	93	ILE
1	G	103	LYS
1	G	107	LYS
1	G	128	LEU
1	G	135	GLU
1	G	141	LYS
1	G	142	ASP
1	G	144	ASN
1	G	146	VAL
1	G	167	SER
1	G	175	SER
1	G	177	ASP
1	G	181	GLU
1	G	193	LYS
1	G	197	VAL
1	G	200	SER
1	G	203	ASN
1	G	207	ILE
1	G	210	THR
1	G	215	LYS
1	G	216	GLU
1	G	227	ILE
1	G	228	GLU
1	G	234	GLU
1	G	240	ILE
1	G	250	ASN
1	G	252	GLN
1	G	269	ARG
1	G	287	GLU
1	G	293	ASN
1	G	316	SER
1	G	322	ARG
1	G	325	SER

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Mol	Chain	Res	Type
1	G	332	MET
1	G	342	ARG
1	G	345	LYS
1	G	356	SER
1	G	359	LEU
1	G	361	VAL
1	G	369	GLU
1	G	376	SER
1	G	377	ARG
1	G	384	LYS
1	G	386	ASP
1	G	389	ARG
1	G	390	GLN
1	G	391	ILE
1	G	398	ASP
1	G	415	SER
1	G	416	LYS
1	G	419	LEU
1	G	420	SER
1	G	427	SER
1	G	430	GLU
1	G	440	LEU
1	G	444	ILE
1	H	29	SER
1	H	32	SER
1	H	54	GLN
1	H	73	MET
1	H	93	ILE
1	H	96	MET
1	H	103	LYS
1	H	107	LYS
1	H	116	ASP
1	H	123	LYS
1	H	138	ARG
1	H	141	LYS
1	H	175	SER
1	H	189	VAL
1	H	192	ASP
1	H	193	LYS
1	H	215	LYS
1	H	216	GLU
1	H	240	ILE

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Mol	Chain	Res	Type
1	H	250	ASN
1	H	269	ARG
1	H	286	SER
1	H	334	LYS
1	H	344	ILE
1	H	355	GLU
1	H	356	SER
1	H	361	VAL
1	H	384	LYS
1	H	385	LYS
1	H	389	ARG
1	H	399	SER
1	H	408	THR
1	H	413	ILE
1	H	433	GLU
1	H	451	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	158	ASN
1	A	250	ASN
1	A	309	ASN
1	A	390	GLN
1	A	445	ASN
1	A	455	HIS
1	B	176	HIS
1	B	217	ASN
1	B	250	ASN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	382	GLN
1	B	422	ASN
1	B	434	ASN
1	B	445	ASN
1	B	448	ASN
1	C	118	GLN
1	C	176	HIS
1	C	217	ASN
1	C	252	GLN

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Mol	Chain	Res	Type
1	C	360	GLN
1	C	401	GLN
1	C	434	ASN
1	D	176	HIS
1	D	247	GLN
1	D	250	ASN
1	D	252	GLN
1	D	360	GLN
1	D	441	GLN
1	D	445	ASN
1	E	118	GLN
1	E	247	GLN
1	E	250	ASN
1	E	397	HIS
1	E	434	ASN
1	E	441	GLN
1	E	445	ASN
1	F	36	ASN
1	F	54	GLN
1	F	118	GLN
1	F	250	ASN
1	F	290	GLN
1	F	292	HIS
1	F	360	GLN
1	F	434	ASN
1	F	455	HIS
1	G	54	GLN
1	G	118	GLN
1	G	143	ASN
1	G	247	GLN
1	G	250	ASN
1	G	401	GLN
1	G	405	HIS
1	G	434	ASN
1	H	247	GLN
1	H	292	HIS
1	H	401	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	BIB	A	2502	-	3,6,6	0.58	0	1,7,7	0.53	0
3	BIB	B	1502	-	3,6,6	0.47	0	1,7,7	0.68	0
3	BIB	C	3502	-	3,6,6	0.48	0	1,7,7	0.15	0
3	BIB	D	4502	-	3,6,6	0.54	0	1,7,7	0.02	0
3	BIB	E	5502	-	3,6,6	0.56	0	1,7,7	0.31	0
3	BIB	E	6502	-	3,6,6	0.56	0	1,7,7	0.30	0
3	BIB	G	7502	-	3,6,6	0.42	0	1,7,7	0.41	0
3	BIB	G	8502	-	3,6,6	0.37	0	1,7,7	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BIB	A	2502	-	-	0/1/6/6	0/0/0/0
3	BIB	B	1502	-	-	0/1/6/6	0/0/0/0
3	BIB	C	3502	-	-	0/1/6/6	0/0/0/0
3	BIB	D	4502	-	-	0/1/6/6	0/0/0/0
3	BIB	E	5502	-	-	0/1/6/6	0/0/0/0
3	BIB	E	6502	-	-	0/1/6/6	0/0/0/0
3	BIB	G	7502	-	-	0/1/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BIB	G	8502	-	-	0/1/6/6	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2502	BIB	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	438/462 (94%)	0.92	62 (14%) 4 3	12, 16, 19, 29	0
1	B	433/462 (93%)	1.11	77 (17%) 2 1	13, 16, 18, 20	0
1	C	438/462 (94%)	0.75	41 (9%) 11 8	13, 16, 19, 30	0
1	D	437/462 (94%)	1.22	95 (21%) 1 1	14, 16, 17, 20	0
1	E	433/462 (93%)	2.32	214 (49%) 0 0	15, 16, 17, 20	0
1	F	438/462 (94%)	0.71	45 (10%) 9 6	13, 16, 19, 31	0
1	G	430/462 (93%)	2.22	212 (49%) 0 0	13, 16, 17, 20	0
1	H	438/462 (94%)	0.87	45 (10%) 9 6	12, 16, 19, 24	0
All	All	3485/3696 (94%)	1.26	791 (22%) 1 1	12, 16, 18, 31	0

All (791) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	211	PRO	9.0
1	G	447	ASP	8.5
1	B	455	HIS	8.5
1	G	55	GLU	8.3
1	E	455	HIS	8.1
1	E	68	ALA	8.1
1	E	176	HIS	8.0
1	E	221	ALA	7.8
1	E	93	ILE	7.6
1	G	455	HIS	7.3
1	E	201	LEU	7.2
1	G	454	GLY	7.2
1	G	50	ALA	7.2
1	G	30	ILE	7.1
1	E	194	PRO	7.1
1	D	455	HIS	6.9

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Mol	Chain	Res	Type	RSRZ
1	G	53	GLY	6.9
1	E	183	ALA	6.8
1	G	386	ASP	6.8
1	G	365	VAL	6.7
1	E	106	GLY	6.7
1	E	25	ALA	6.6
1	D	19	THR	6.6
1	E	212	ALA	6.6
1	G	394	GLY	6.5
1	E	178	LEU	6.4
1	E	177	ASP	6.4
1	G	370	VAL	6.3
1	E	103	LYS	6.3
1	E	192	ASP	6.3
1	E	76	TRP	6.3
1	E	163	ARG	6.2
1	E	451	VAL	6.2
1	G	377	ARG	6.2
1	E	110	ALA	6.2
1	E	204	ILE	6.1
1	E	199	ASP	6.0
1	G	104	ASN	6.0
1	E	100	TYR	6.0
1	G	444	ILE	6.0
1	G	383	PHE	5.9
1	G	368	HIS	5.9
1	E	91	ASP	5.9
1	D	23	PRO	5.8
1	B	25	ALA	5.8
1	G	452	ILE	5.7
1	E	449	TYR	5.7
1	G	363	PRO	5.7
1	G	396	GLY	5.6
1	G	412	PHE	5.6
1	G	373	GLU	5.6
1	G	364	ALA	5.5
1	E	92	LYS	5.5
1	E	39	ILE	5.5
1	B	192	ASP	5.4
1	E	96	MET	5.4
1	G	388	VAL	5.4
1	D	381	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	30	ILE	5.3
1	E	86	CYS	5.3
1	D	54	GLN	5.3
1	E	193	LYS	5.3
1	H	87	LYS	5.3
1	G	426	TYR	5.2
1	G	451	VAL	5.2
1	F	455	HIS	5.2
1	D	192	ASP	5.2
1	E	101	PRO	5.2
1	D	21	ASN	5.2
1	G	31	ALA	5.2
1	D	451	VAL	5.2
1	E	41	GLU	5.2
1	E	152	CYS	5.1
1	G	453	ARG	5.1
1	C	18	GLY	5.1
1	E	104	ASN	5.1
1	G	443	ILE	5.1
1	D	190	GLY	5.1
1	E	404	PRO	5.1
1	E	365	VAL	5.0
1	G	384	LYS	5.0
1	H	19	THR	5.0
1	G	223	PHE	5.0
1	E	149	TYR	5.0
1	E	210	THR	5.0
1	E	219	ILE	5.0
1	E	43	GLY	4.9
1	F	19	THR	4.9
1	E	180	LEU	4.9
1	E	24	ALA	4.9
1	E	70	ASP	4.9
1	D	55	GLU	4.9
1	G	27	PRO	4.9
1	E	79	ASN	4.9
1	E	197	VAL	4.9
1	B	54	GLN	4.9
1	G	369	GLU	4.8
1	E	454	GLY	4.8
1	G	100	TYR	4.8
1	E	69	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	26	ALA	4.8
1	E	142	ASP	4.8
1	E	368	HIS	4.8
1	E	405	HIS	4.8
1	D	178	LEU	4.8
1	G	230	GLY	4.8
1	E	174	TRP	4.7
1	D	193	LYS	4.7
1	G	436	PHE	4.7
1	G	395	ALA	4.7
1	E	185	GLY	4.7
1	G	112	GLY	4.7
1	G	32	SER	4.7
1	A	298	CYS	4.7
1	E	191	GLU	4.7
1	B	104	ASN	4.7
1	E	55	GLU	4.7
1	G	33	GLY	4.7
1	G	327	ASP	4.6
1	E	98	ALA	4.6
1	E	33	GLY	4.6
1	H	454	GLY	4.6
1	E	102	GLY	4.6
1	E	366	ASN	4.6
1	G	56	SER	4.6
1	B	47	GLY	4.5
1	G	29	SER	4.5
1	E	214	TYR	4.5
1	D	454	GLY	4.5
1	B	194	PRO	4.5
1	E	207	ILE	4.5
1	H	455	HIS	4.5
1	E	182	GLU	4.5
1	D	20	LEU	4.5
1	G	192	ASP	4.5
1	G	385	LYS	4.5
1	G	323	HIS	4.5
1	E	105	GLY	4.5
1	E	56	SER	4.5
1	D	104	ASN	4.4
1	B	30	ILE	4.4
1	G	43	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	102	GLY	4.4
1	E	99	VAL	4.4
1	G	408	THR	4.4
1	E	198	TYR	4.4
1	C	298	CYS	4.4
1	G	334	LYS	4.4
1	B	454	GLY	4.3
1	E	87	LYS	4.3
1	E	88	VAL	4.3
1	D	56	SER	4.3
1	E	181	GLU	4.3
1	D	50	ALA	4.3
1	E	53	GLY	4.3
1	A	129	GLY	4.3
1	B	452	ILE	4.3
1	E	139	THR	4.3
1	E	138	ARG	4.3
1	E	377	ARG	4.2
1	G	235	ASP	4.2
1	G	366	ASN	4.2
1	G	149	TYR	4.2
1	C	133	GLY	4.2
1	D	87	LYS	4.2
1	E	184	TYR	4.2
1	G	54	GLN	4.2
1	G	246	VAL	4.2
1	F	18	GLY	4.2
1	G	111	THR	4.2
1	E	48	GLY	4.1
1	E	386	ASP	4.1
1	E	54	GLN	4.1
1	G	392	TRP	4.1
1	B	86	CYS	4.1
1	C	192	ASP	4.1
1	D	24	ALA	4.1
1	E	369	GLU	4.1
1	C	129	GLY	4.1
1	G	380	PHE	4.1
1	E	187	MET	4.1
1	F	129	GLY	4.1
1	D	31	ALA	4.1
1	E	95	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	128	LEU	4.1
1	A	152	CYS	4.1
1	E	164	PHE	4.0
1	G	367	PHE	4.0
1	D	142	ASP	4.0
1	E	52	TRP	4.0
1	G	193	LYS	4.0
1	G	381	ALA	4.0
1	E	120	GLU	4.0
1	H	348	ASP	4.0
1	E	121	ALA	4.0
1	E	367	PHE	4.0
1	E	118	GLN	4.0
1	G	249	TYR	4.0
1	E	150	ASP	4.0
1	G	231	PRO	3.9
1	E	73	MET	3.9
1	B	451	VAL	3.9
1	E	162	ALA	3.9
1	G	414	PRO	3.9
1	E	190	GLY	3.9
1	D	146	VAL	3.9
1	H	120	GLU	3.9
1	E	206	TYR	3.9
1	E	84	LEU	3.9
1	G	433	GLU	3.9
1	G	432	ILE	3.9
1	G	152	CYS	3.9
1	D	79	ASN	3.9
1	G	103	LYS	3.9
1	G	41	GLU	3.8
1	A	455	HIS	3.8
1	G	404	PRO	3.8
1	E	97	PHE	3.8
1	G	430	GLU	3.8
1	E	90	VAL	3.8
1	E	189	VAL	3.8
1	E	220	ASP	3.8
1	G	144	ASN	3.8
1	G	57	HIS	3.8
1	G	239	ALA	3.8
1	B	105	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLY	3.8
1	G	441	GLN	3.8
1	G	51	ARG	3.7
1	E	151	VAL	3.7
1	G	393	SER	3.7
1	G	448	ASN	3.7
1	D	22	LEU	3.7
1	F	128	LEU	3.7
1	E	450	ARG	3.7
1	G	402	THR	3.7
1	A	132	ALA	3.7
1	B	177	ASP	3.7
1	E	75	ASP	3.7
1	H	192	ASP	3.7
1	F	130	VAL	3.7
1	G	424	TYR	3.7
1	E	385	LYS	3.7
1	A	111	THR	3.7
1	B	68	ALA	3.6
1	B	275	LEU	3.6
1	C	455	HIS	3.6
1	H	130	VAL	3.6
1	E	423	TYR	3.6
1	E	424	TYR	3.6
1	E	126	GLY	3.6
1	C	130	VAL	3.6
1	E	200	SER	3.6
1	E	400	CYS	3.6
1	D	199	ASP	3.6
1	B	53	GLY	3.6
1	E	67	THR	3.6
1	D	32	SER	3.6
1	E	370	VAL	3.6
1	B	100	TYR	3.6
1	E	46	PHE	3.6
1	D	135	GLU	3.6
1	F	190	GLY	3.6
1	G	113	SER	3.5
1	A	223	PHE	3.5
1	E	165	ALA	3.5
1	D	52	TRP	3.5
1	A	131	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	128	LEU	3.5
1	D	120	GLU	3.5
1	G	59	PHE	3.5
1	A	126	GLY	3.5
1	H	18	GLY	3.5
1	E	179	SER	3.5
1	B	149	TYR	3.5
1	G	145	TYR	3.5
1	E	44	SER	3.4
1	A	127	ILE	3.4
1	E	109	THR	3.4
1	F	225	LEU	3.4
1	B	369	GLU	3.4
1	E	364	ALA	3.4
1	E	170	GLY	3.4
1	G	143	ASN	3.4
1	G	190	GLY	3.4
1	D	30	ILE	3.4
1	C	155	VAL	3.4
1	E	23	PRO	3.4
1	G	58	GLU	3.4
1	A	130	VAL	3.4
1	G	177	ASP	3.4
1	G	417	ASP	3.4
1	G	81	CYS	3.4
1	E	384	LYS	3.4
1	F	189	VAL	3.4
1	G	52	TRP	3.4
1	E	453	ARG	3.4
1	D	221	ALA	3.4
1	E	45	GLN	3.4
1	E	433	GLU	3.4
1	G	228	GLU	3.4
1	G	362	SER	3.4
1	C	132	ALA	3.4
1	B	32	SER	3.4
1	G	449	TYR	3.3
1	G	331	THR	3.3
1	G	411	ILE	3.3
1	D	384	LYS	3.3
1	C	299	GLY	3.3
1	G	87	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	227	ILE	3.3
1	G	440	LEU	3.3
1	E	402	THR	3.3
1	G	379	ALA	3.3
1	A	439	LEU	3.3
1	A	275	LEU	3.3
1	D	191	GLU	3.3
1	E	235	ASP	3.3
1	G	245	GLY	3.3
1	E	224	GLU	3.2
1	D	198	TYR	3.2
1	B	87	LYS	3.2
1	H	298	CYS	3.2
1	F	127	ILE	3.2
1	F	298	CYS	3.2
1	B	179	SER	3.2
1	E	169	THR	3.2
1	H	132	ALA	3.2
1	C	127	ILE	3.2
1	G	390	GLN	3.2
1	E	381	ALA	3.2
1	G	139	THR	3.2
1	F	152	CYS	3.2
1	E	452	ILE	3.2
1	G	101	PRO	3.2
1	B	31	ALA	3.2
1	C	115	LEU	3.1
1	B	101	PRO	3.1
1	A	225	LEU	3.1
1	A	411	ILE	3.1
1	E	40	LEU	3.1
1	E	186	LEU	3.1
1	G	151	VAL	3.1
1	A	299	GLY	3.1
1	D	68	ALA	3.1
1	E	77	PHE	3.1
1	E	223	PHE	3.1
1	G	181	GLU	3.1
1	A	133	GLY	3.1
1	C	126	GLY	3.1
1	C	278	SER	3.1
1	H	129	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	193	LYS	3.1
1	A	192	ASP	3.1
1	H	127	ILE	3.1
1	D	33	GLY	3.1
1	G	375	VAL	3.1
1	G	335	GLU	3.1
1	B	203	ASN	3.1
1	C	223	PHE	3.1
1	C	327	ASP	3.1
1	E	327	ASP	3.1
1	G	374	CYS	3.1
1	A	155	VAL	3.1
1	B	181	GLU	3.1
1	E	447	ASP	3.1
1	G	182	GLU	3.1
1	E	72	ALA	3.1
1	F	165	ALA	3.1
1	G	431	GLU	3.1
1	E	108	PRO	3.0
1	E	246	VAL	3.0
1	G	146	VAL	3.0
1	G	214	TYR	3.0
1	H	153	VAL	3.0
1	B	453	ARG	3.0
1	A	318	THR	3.0
1	E	115	LEU	3.0
1	G	148	ASN	3.0
1	G	225	LEU	3.0
1	G	86	CYS	3.0
1	E	215	LYS	3.0
1	G	99	VAL	3.0
1	C	19	THR	3.0
1	D	202	LYS	3.0
1	E	37	GLN	3.0
1	E	81	CYS	3.0
1	B	377	ARG	3.0
1	F	115	LEU	3.0
1	G	355	GLU	3.0
1	G	382	GLN	3.0
1	D	41	GLU	3.0
1	F	454	GLY	3.0
1	G	178	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	111	THR	3.0
1	A	279	SER	3.0
1	E	380	PHE	3.0
1	D	49	VAL	3.0
1	D	335	GLU	3.0
1	E	374	CYS	3.0
1	G	129	GLY	3.0
1	H	126	GLY	3.0
1	F	132	ALA	3.0
1	A	317	PHE	3.0
1	D	369	GLU	3.0
1	E	202	LYS	3.0
1	A	154	VAL	3.0
1	E	208	GLY	3.0
1	F	154	VAL	3.0
1	G	105	GLY	3.0
1	E	26	ALA	3.0
1	B	103	LYS	3.0
1	B	51	ARG	2.9
1	E	134	LEU	2.9
1	A	278	SER	2.9
1	B	56	SER	2.9
1	E	71	GLY	2.9
1	D	105	GLY	2.9
1	H	264	GLY	2.9
1	C	154	VAL	2.9
1	G	153	VAL	2.9
1	E	175	SER	2.9
1	F	192	ASP	2.9
1	G	419	LEU	2.9
1	G	241	GLY	2.9
1	G	215	LYS	2.9
1	G	391	ILE	2.9
1	D	392	TRP	2.9
1	F	131	LEU	2.8
1	G	226	HIS	2.8
1	D	101	PRO	2.8
1	G	240	ILE	2.8
1	G	138	ARG	2.8
1	A	443	ILE	2.8
1	F	275	LEU	2.8
1	G	203	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	211	PRO	2.8
1	E	216	GLU	2.8
1	G	387	GLN	2.8
1	A	282	ILE	2.8
1	C	131	LEU	2.8
1	A	153	VAL	2.8
1	C	317	PHE	2.8
1	F	317	PHE	2.8
1	G	202	LYS	2.8
1	G	238	LYS	2.8
1	G	220	ASP	2.8
1	C	153	VAL	2.8
1	A	110	ALA	2.8
1	E	89	LYS	2.8
1	E	448	ASN	2.8
1	G	437	LYS	2.8
1	D	66	GLY	2.8
1	H	443	ILE	2.8
1	D	34	ARG	2.8
1	F	111	THR	2.8
1	C	225	LEU	2.8
1	G	34	ARG	2.8
1	G	389	ARG	2.8
1	E	148	ASN	2.8
1	E	383	PHE	2.8
1	D	83	SER	2.7
1	E	129	GLY	2.8
1	G	106	GLY	2.8
1	B	281	MET	2.7
1	G	61	MET	2.7
1	G	328	VAL	2.7
1	D	203	ASN	2.7
1	B	386	ASP	2.7
1	D	102	GLY	2.7
1	E	82	GLU	2.7
1	E	83	SER	2.7
1	D	440	LEU	2.7
1	G	438	VAL	2.7
1	E	107	LYS	2.7
1	F	318	THR	2.7
1	B	42	THR	2.7
1	E	375	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	82	GLU	2.7
1	E	32	SER	2.7
1	A	20	LEU	2.7
1	G	176	HIS	2.7
1	G	191	GLU	2.7
1	G	446	TYR	2.7
1	B	278	SER	2.7
1	B	276	LEU	2.7
1	C	152	CYS	2.7
1	E	205	GLY	2.7
1	F	133	GLY	2.7
1	G	150	ASP	2.7
1	D	103	LYS	2.7
1	G	107	LYS	2.7
1	G	80	GLU	2.7
1	D	53	GLY	2.7
1	E	406	VAL	2.7
1	F	443	ILE	2.7
1	G	198	TYR	2.7
1	B	24	ALA	2.7
1	E	397	HIS	2.6
1	B	327	ASP	2.6
1	D	47	GLY	2.6
1	F	348	ASP	2.6
1	F	136	VAL	2.6
1	G	49	VAL	2.6
1	G	410	MET	2.6
1	E	401	GLN	2.6
1	D	144	ASN	2.6
1	E	122	GLY	2.6
1	H	439	LEU	2.6
1	G	434	ASN	2.6
1	D	209	ASP	2.6
1	G	326	ASP	2.6
1	F	113	SER	2.6
1	G	109	THR	2.6
1	C	112	GLY	2.6
1	G	69	LEU	2.6
1	B	114	HIS	2.6
1	G	85	GLY	2.6
1	B	441	GLN	2.6
1	D	71	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	126	GLY	2.6
1	D	177	ASP	2.6
1	E	156	TRP	2.6
1	E	196	SER	2.6
1	A	115	LEU	2.6
1	C	318	THR	2.6
1	E	209	ASP	2.6
1	G	76	TRP	2.6
1	B	46	PHE	2.6
1	D	377	ARG	2.5
1	C	113	SER	2.5
1	F	155	VAL	2.5
1	G	180	LEU	2.5
1	D	147	PRO	2.5
1	E	27	PRO	2.5
1	B	373	GLU	2.5
1	G	122	GLY	2.5
1	G	429	PRO	2.5
1	F	153	VAL	2.5
1	G	169	THR	2.5
1	H	331	THR	2.5
1	G	257	HIS	2.5
1	D	187	MET	2.5
1	B	23	PRO	2.5
1	B	55	GLU	2.5
1	E	217	ASN	2.5
1	E	379	ALA	2.5
1	E	444	ILE	2.5
1	G	405	HIS	2.5
1	E	145	TYR	2.5
1	G	187	MET	2.5
1	A	112	GLY	2.5
1	A	300	ILE	2.5
1	B	88	VAL	2.5
1	E	275	LEU	2.5
1	E	440	LEU	2.5
1	F	439	LEU	2.5
1	E	66	GLY	2.5
1	F	223	PHE	2.5
1	G	174	TRP	2.5
1	A	301	ILE	2.5
1	G	154	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	128	LEU	2.5
1	A	113	SER	2.5
1	D	106	GLY	2.5
1	D	249	TYR	2.5
1	D	327	ASP	2.5
1	G	79	ASN	2.5
1	G	348	ASP	2.5
1	G	372	ILE	2.4
1	E	172	SER	2.4
1	B	214	TYR	2.4
1	A	440	LEU	2.4
1	A	151	VAL	2.4
1	A	432	ILE	2.4
1	C	114	HIS	2.4
1	G	397	HIS	2.4
1	E	213	SER	2.4
1	G	126	GLY	2.4
1	E	225	LEU	2.4
1	G	218	GLU	2.4
1	G	236	GLU	2.4
1	G	439	LEU	2.4
1	D	189	VAL	2.4
1	D	219	ILE	2.4
1	E	29	SER	2.4
1	G	415	SER	2.4
1	A	218	GLU	2.4
1	B	206	TYR	2.4
1	B	449	TYR	2.4
1	E	49	VAL	2.4
1	E	111	THR	2.4
1	G	255	THR	2.4
1	H	113	SER	2.4
1	G	445	ASN	2.4
1	E	407	PRO	2.4
1	G	121	ALA	2.4
1	A	114	HIS	2.4
1	A	409	SER	2.4
1	B	187	MET	2.4
1	D	37	GLN	2.4
1	C	439	LEU	2.4
1	D	275	LEU	2.4
1	E	147	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	146	VAL	2.4
1	H	154	VAL	2.4
1	B	279	SER	2.4
1	G	400	CYS	2.4
1	H	191	GLU	2.4
1	C	209	ASP	2.4
1	C	440	LEU	2.4
1	H	131	LEU	2.4
1	A	297	THR	2.4
1	A	453	ARG	2.4
1	D	81	CYS	2.4
1	H	223	PHE	2.3
1	B	71	GLY	2.3
1	E	245	GLY	2.3
1	G	185	GLY	2.3
1	G	435	GLY	2.3
1	D	449	TYR	2.3
1	A	136	VAL	2.3
1	B	175	SER	2.3
1	E	51	ARG	2.3
1	E	62	ARG	2.3
1	C	297	THR	2.3
1	D	46	PHE	2.3
1	D	185	GLY	2.3
1	H	115	LEU	2.3
1	B	26	ALA	2.3
1	F	110	ALA	2.3
1	B	189	VAL	2.3
1	F	209	ASP	2.3
1	A	19	THR	2.3
1	E	58	GLU	2.3
1	A	134	LEU	2.3
1	F	299	GLY	2.3
1	H	215	LYS	2.3
1	C	279	SER	2.3
1	D	362	SER	2.3
1	H	155	VAL	2.3
1	B	204	ILE	2.3
1	C	443	ILE	2.3
1	E	61	MET	2.3
1	E	274	ALA	2.3
1	H	222	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLU	2.3
1	E	80	GLU	2.3
1	G	78	THR	2.3
1	G	47	GLY	2.3
1	G	60	GLY	2.3
1	A	209	ASP	2.3
1	B	75	ASP	2.3
1	B	366	ASN	2.3
1	D	423	TYR	2.3
1	G	244	THR	2.3
1	E	161	GLY	2.3
1	D	179	SER	2.3
1	D	138	ARG	2.3
1	G	360	GLN	2.3
1	A	216	GLU	2.3
1	E	236	GLU	2.3
1	H	409	SER	2.3
1	E	222	HIS	2.3
1	G	248	ALA	2.3
1	G	232	ILE	2.3
1	A	319	LEU	2.2
1	D	216	GLU	2.2
1	C	315	VAL	2.2
1	E	112	GLY	2.2
1	F	278	SER	2.2
1	B	50	ALA	2.2
1	B	205	GLY	2.2
1	B	274	ALA	2.2
1	G	68	ALA	2.2
1	A	191	GLU	2.2
1	D	182	GLU	2.2
1	G	84	LEU	2.2
1	D	348	ASP	2.2
1	A	316	SER	2.2
1	G	250	ASN	2.2
1	D	162	ALA	2.2
1	E	410	MET	2.2
1	E	392	TRP	2.2
1	H	318	THR	2.2
1	E	64	LEU	2.2
1	G	233	LEU	2.2
1	C	110	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	438	VAL	2.2
1	E	74	ARG	2.2
1	E	346	ILE	2.2
1	F	301	ILE	2.2
1	H	150	ASP	2.2
1	B	120	GLU	2.2
1	G	294	GLY	2.2
1	H	112	GLY	2.2
1	A	315	VAL	2.2
1	H	189	VAL	2.2
1	D	386	ASP	2.2
1	D	45	GLN	2.2
1	E	168	CYS	2.2
1	A	442	ALA	2.2
1	A	156	TRP	2.2
1	B	430	GLU	2.2
1	G	40	LEU	2.2
1	G	128	LEU	2.2
1	B	148	ASN	2.2
1	E	94	GLY	2.2
1	D	72	ALA	2.2
1	D	364	ALA	2.2
1	E	373	GLU	2.2
1	G	82	GLU	2.2
1	F	39	ILE	2.1
1	G	413	ILE	2.1
1	B	312	PRO	2.1
1	D	237	ASN	2.1
1	D	404	PRO	2.1
1	D	429	PRO	2.1
1	E	203	ASN	2.1
1	D	181	GLU	2.1
1	H	110	ALA	2.1
1	B	199	ASP	2.1
1	E	441	GLN	2.1
1	G	37	GLN	2.1
1	A	109	THR	2.1
1	F	411	ILE	2.1
1	G	219	ILE	2.1
1	G	287	GLU	2.1
1	G	110	ALA	2.1
1	H	327	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	153	VAL	2.1
1	G	376	SER	2.1
1	G	409	SER	2.1
1	B	156	TRP	2.1
1	H	86	CYS	2.1
1	G	36	ASN	2.1
1	A	65	ALA	2.1
1	A	190	GLY	2.1
1	B	308	VAL	2.1
1	C	316	SER	2.1
1	G	28	LEU	2.1
1	D	51	ARG	2.1
1	E	34	ARG	2.1
1	B	182	GLU	2.1
1	H	317	PHE	2.1
1	D	129	GLY	2.1
1	B	191	GLU	2.1
1	D	311	ILE	2.1
1	F	114	HIS	2.1
1	A	224	GLU	2.1
1	C	156	TRP	2.1
1	H	436	PHE	2.1
1	B	81	CYS	2.1
1	D	62	ARG	2.1
1	G	165	ALA	2.1
1	H	263	ALA	2.1
1	D	246	VAL	2.1
1	E	130	VAL	2.1
1	E	387	GLN	2.1
1	D	108	PRO	2.1
1	E	429	PRO	2.1
1	C	111	THR	2.0
1	B	215	LYS	2.0
1	B	380	PHE	2.0
1	A	222	HIS	2.0
1	C	319	LEU	2.0
1	E	113	SER	2.0
1	E	248	ALA	2.0
1	F	279	SER	2.0
1	G	212	ALA	2.0
1	G	38	THR	2.0
1	A	281	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	444	ILE	2.0
1	D	452	ILE	2.0
1	E	127	ILE	2.0
1	F	296	PHE	2.0
1	G	398	ASP	2.0
1	H	190	GLY	2.0
1	B	193	LYS	2.0
1	D	276	LEU	2.0
1	G	423	TYR	2.0
1	H	225	LEU	2.0
1	B	365	VAL	2.0
1	F	151	VAL	2.0
1	F	375	VAL	2.0
1	G	406	VAL	2.0
1	H	411	ILE	2.0
1	E	57	HIS	2.0
1	E	50	ALA	2.0
1	E	143	ASN	2.0
1	G	224	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BIB	E	6502	7/7	0.82	0.27	3.57	21,22,24,24	0
3	BIB	G	8502	7/7	0.69	0.32	3.03	19,21,21,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BIB	C	3502	7/7	0.89	0.25	1.62	24,26,27,27	0
3	BIB	E	5502	7/7	0.85	0.30	1.59	16,17,18,18	0
3	BIB	D	4502	7/7	0.80	0.26	0.86	16,16,17,17	0
3	BIB	G	7502	7/7	0.78	0.33	-0.03	12,13,15,15	0
3	BIB	B	1502	7/7	0.86	0.23	-0.09	19,23,24,25	0
3	BIB	A	2502	7/7	0.85	0.20	-0.36	15,19,21,21	0
2	ZN	A	500	1/1	1.00	0.21	-0.82	15,15,15,15	0
2	ZN	C	500	1/1	0.98	0.18	-1.09	16,16,16,16	0
2	ZN	F	500	1/1	0.98	0.17	-1.23	16,16,16,16	0
2	ZN	C	501	1/1	0.98	0.15	-1.41	18,18,18,18	0
2	ZN	H	500	1/1	0.98	0.14	-1.54	15,15,15,15	0
2	ZN	A	501	1/1	0.99	0.15	-1.68	18,18,18,18	0
2	ZN	F	501	1/1	0.97	0.13	-1.82	18,18,18,18	0
2	ZN	B	500	1/1	0.96	0.11	-2.00	16,16,16,16	0
2	ZN	H	501	1/1	0.93	0.13	-2.10	18,18,18,18	0
2	ZN	D	500	1/1	0.93	0.08	-2.59	15,15,15,15	0
2	ZN	B	501	1/1	0.93	0.06	-2.63	18,18,18,18	0
2	ZN	E	500	1/1	0.84	0.06	-2.82	16,16,16,16	0
2	ZN	G	501	1/1	0.94	0.14	-2.94	17,17,17,17	0
2	ZN	D	501	1/1	0.92	0.07	-3.01	18,18,18,18	0
2	ZN	G	500	1/1	0.95	0.05	-3.11	15,15,15,15	0
2	ZN	E	501	1/1	0.91	0.08	-3.97	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.