



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:09 AM UTC

PDB ID : 1R3N / pdb_00001r3n
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri*
Authors : Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritsch, 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

<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:

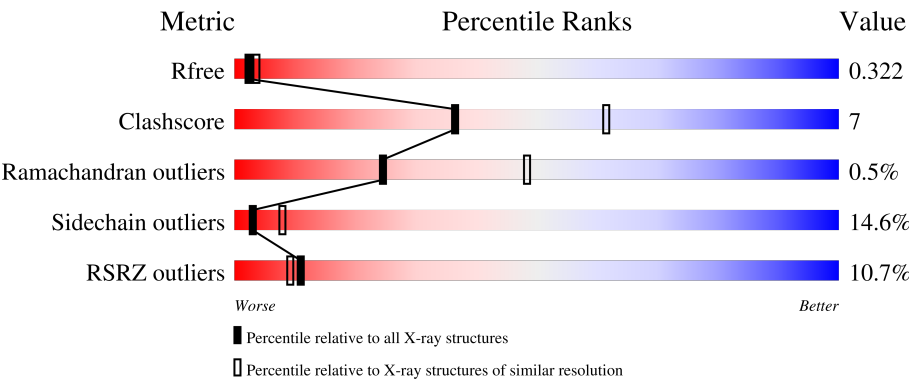
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	462	11% 75% 17% • 5%
1	B	462	7% 72% 20% • 6%
1	C	462	5% 76% 16% • 5%
1	D	462	5% 72% 20% • 5%
1	E	462	25% 63% 26% 5% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	462	4% 76% 17% 5%
1	G	462	17% 64% 25% 7%
1	H	462	7% 75% 17% 5%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

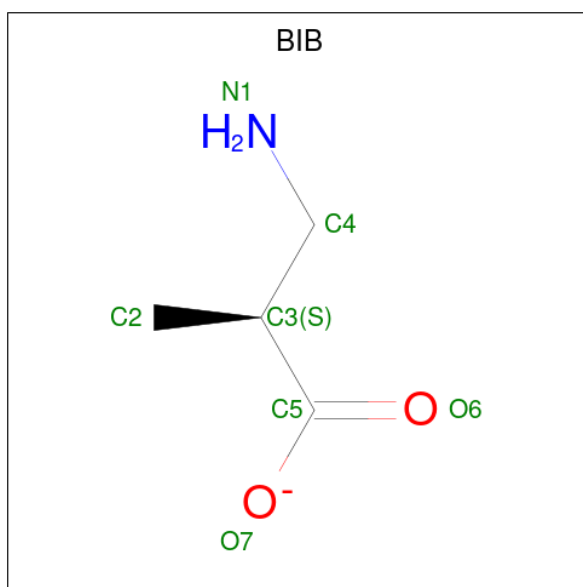
Continued from previous page...

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is BETA-AMINO ISOBUTYRATE (CCD ID: BIB) (formula: C₄H₈NO₂).



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

- Molecule 4 is water.

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

Continued on next page...

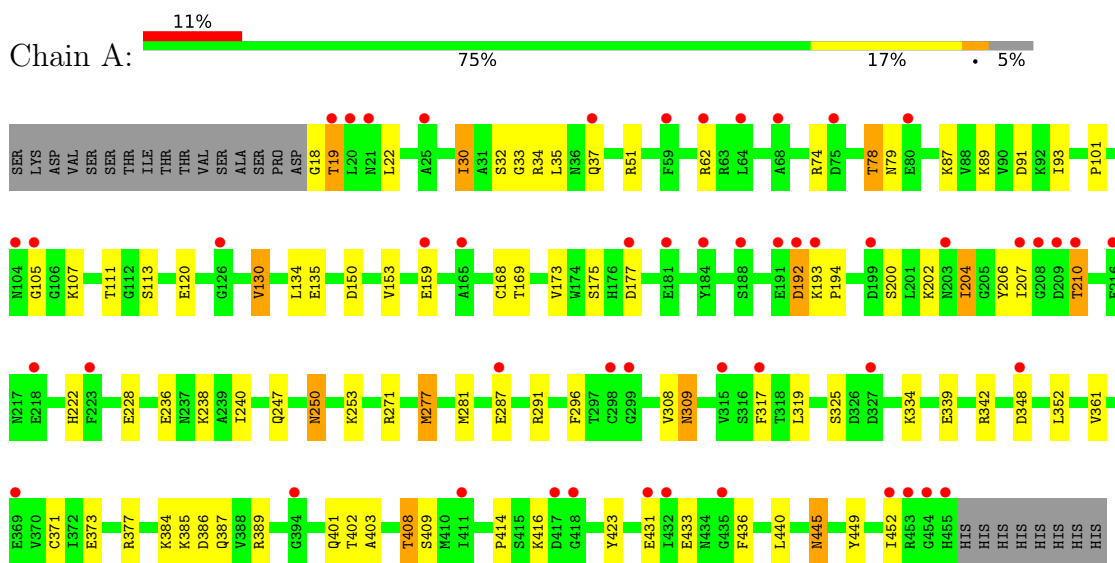
Continued from previous page...

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

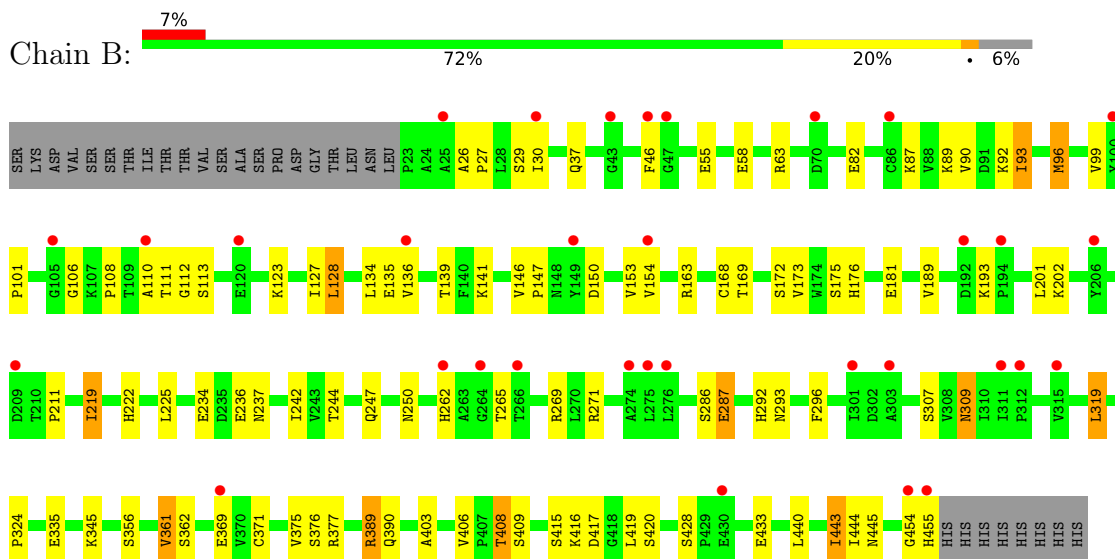
3 Residue-property plots [i](#)

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: beta-alanine synthase

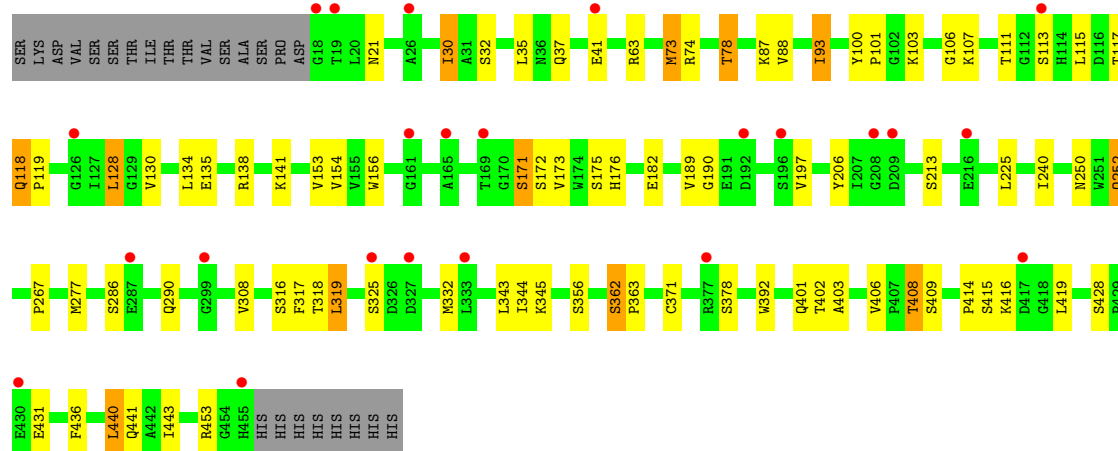


- Molecule 1: beta-alanine synthase



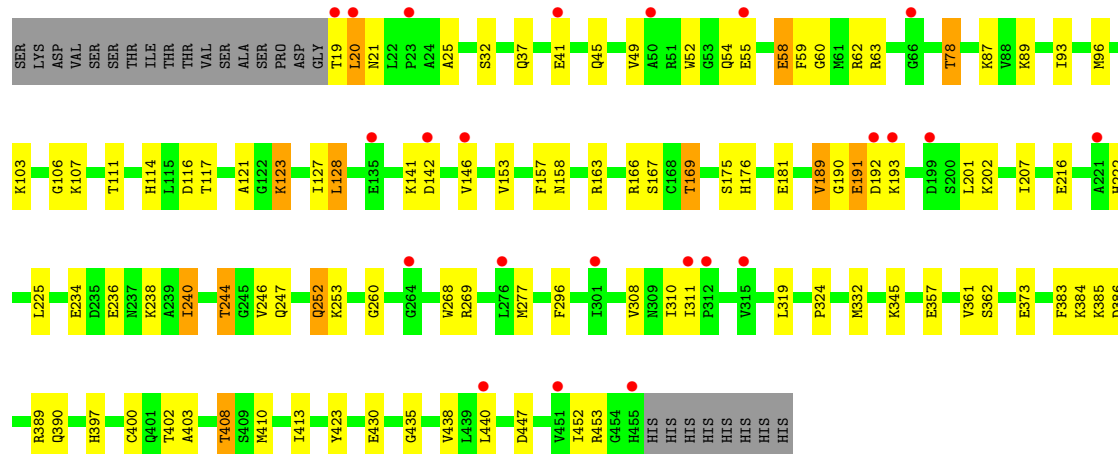
- Molecule 1: beta-alanine synthase

Chain C: 



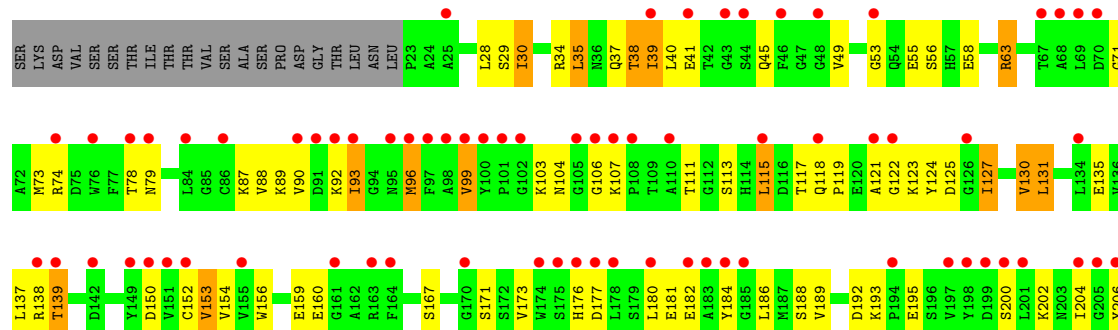
• Molecule 1: beta-alanine synthase

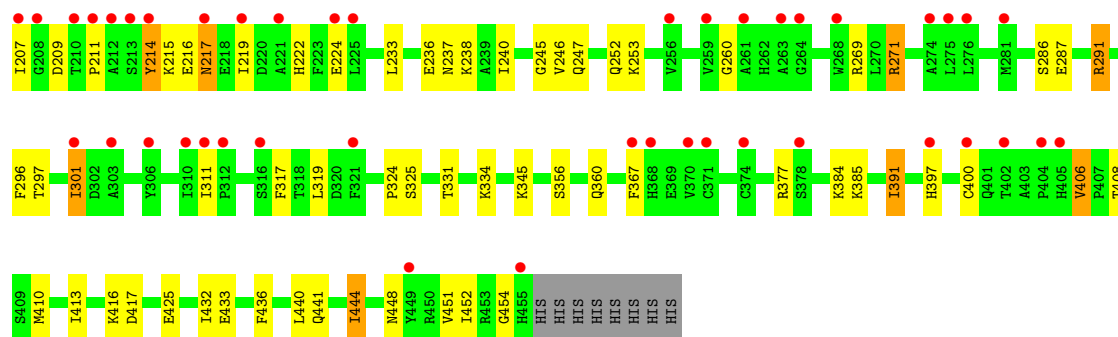
Chain D: 



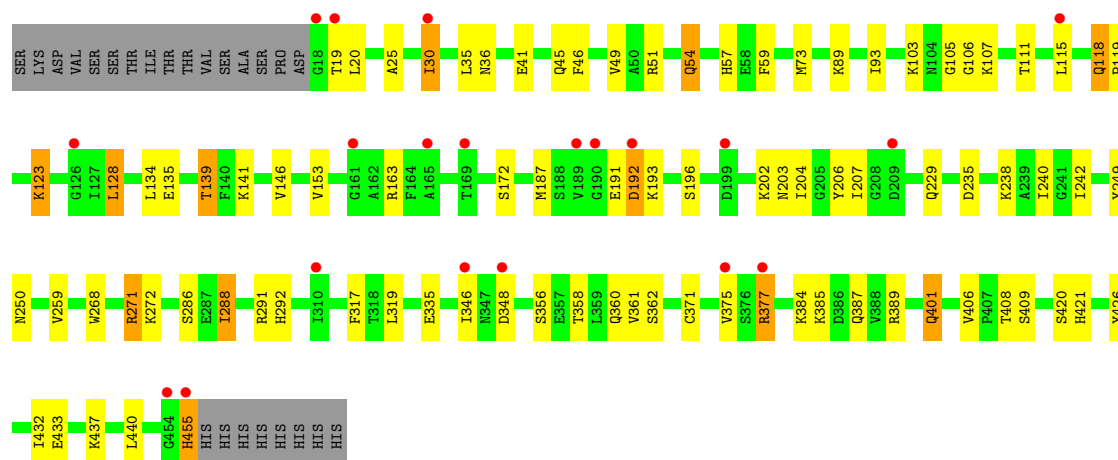
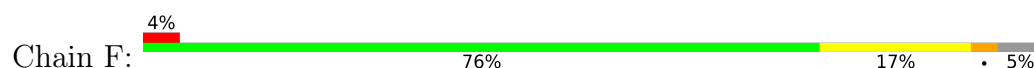
• Molecule 1: beta-alanine synthase

Chain E: 

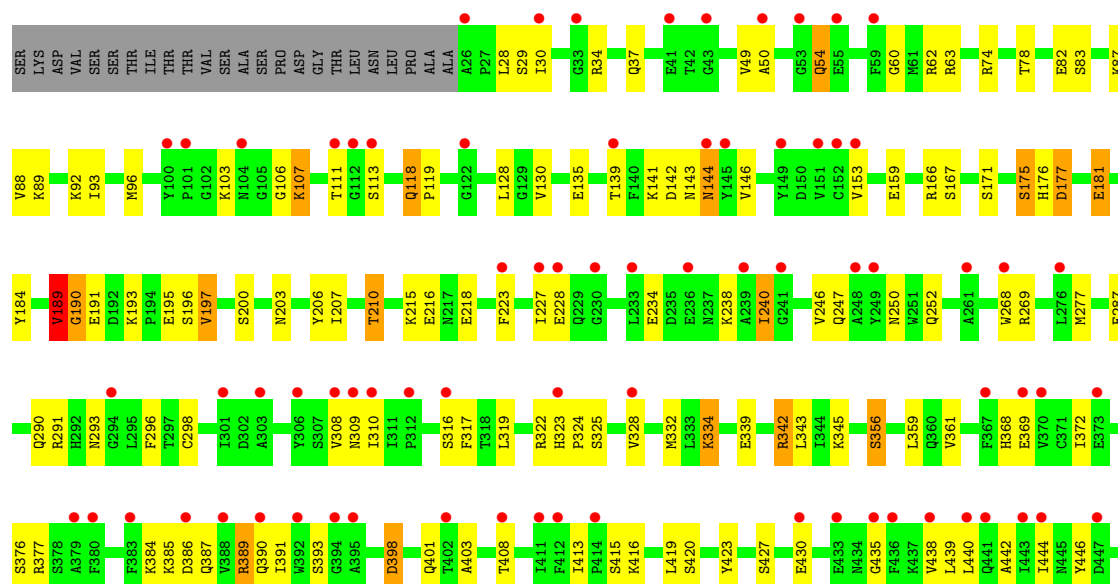


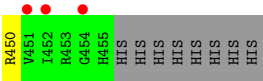


• Molecule 1: beta-alanine synthase

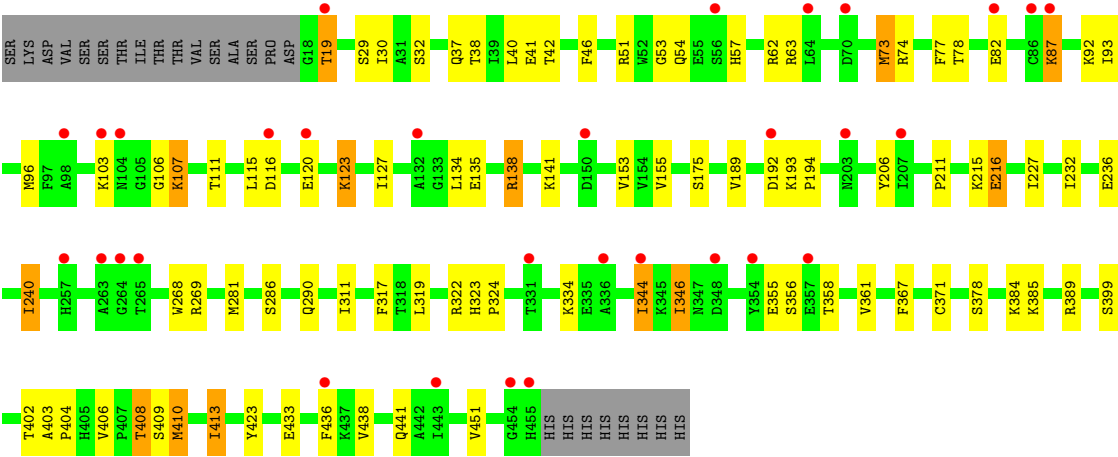
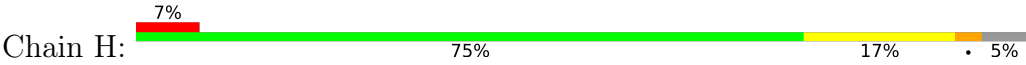


• Molecule 1: beta-alanine synthase





● Molecule 1: beta-alanine synthase



4 Data and refinement statistics

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 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-2.70) 95.7 (25.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.266 0.292 , 0.322	Depositor DCC
R_{free} test set	5296 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 12.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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	0.67	2/3457 (0.1%)	0.96	5/4689 (0.1%)
1	B	0.54	0/3422	0.88	1/4640 (0.0%)
1	C	0.61	0/3457	0.91	0/4689
1	D	0.53	0/3453	0.89	0/4684
1	E	0.48	0/3422	0.88	0/4640
1	F	0.59	0/3457	0.90	1/4689 (0.0%)
1	G	0.49	0/3404	0.88	1/4615 (0.0%)
1	H	0.55	0/3457	0.90	1/4689 (0.0%)
All	All	0.56	2/27529 (0.0%)	0.90	9/37335 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLY	C-O	-9.42	1.08	1.24
1	A	277	MET	SD-CE	-7.65	1.60	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLY	CA-C-O	-9.63	109.72	118.77
1	A	309	ASN	CB-CA-C	-7.87	94.61	109.72
1	B	309	ASN	N-CA-CB	-7.03	100.05	110.53
1	G	309	ASN	CB-CA-C	-6.32	96.73	109.55
1	A	105	GLY	N-CA-C	6.31	126.35	116.01
1	A	19	THR	N-CA-C	-6.23	106.28	114.31
1	H	19	THR	N-CA-C	5.68	118.95	111.28
1	A	105	GLY	O-C-N	-5.41	116.89	122.51
1	F	426	TYR	N-CA-C	5.22	117.87	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3379	0	3264	51	0
1	B	3344	0	3227	41	1
1	C	3379	0	3264	46	0
1	D	3375	0	3261	41	0
1	E	3344	0	3227	74	0
1	F	3379	0	3264	43	0
1	G	3327	0	3209	53	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	382	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 (382) 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
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:N	1:F:455:HIS:CD2	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:D:78:THR:HG22	1:D:96:MET:HE1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:371:CYS:HB3	1:A:409:SER:HB2	1.77	0.67
1:D:189:VAL:CG2	1:D:190:GLY:H	2.06	0.67
1:E:269:ARG:NH2	1:F:235:ASP:OD1	2.26	0.67
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:C:182:GLU:OE1	4:C:3559:HOH:O	2.12	0.66
1:D:244:THR:O	4:D:4531:HOH:O	2.14	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:HG13	1:E:88:VAL:O	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:E:63:ARG:HH12	1:E:115:LEU:HB3	1.65	0.60
1:F:118:GLN:HG3	1:F:119:PRO:HD3	1.82	0.60
1:C:277:MET:HE3	1:C:344:ILE:HA	1.82	0.60
1:E:118:GLN:HG3	1:E:119:PRO:CD	2.24	0.60
1:A:277:MET:HE2	1:A:281:MET:HE3	1.82	0.60
1:C:128:LEU:HD13	1:C:225:LEU:HG	1.83	0.60
1:E:30:ILE:HG21	1:E:436:PHE:HE2	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:317:PHE:CE1	1:E:319:LEU:HD21	2.38	0.59
1:F:25:ALA:O	4:F:576:HOH:O	2.17	0.59
1:B:128:LEU:HD13	1:B:225:LEU:HG	1.83	0.59
1:D:413:ILE:HD11	1:D:435:GLY:HA3	1.83	0.59
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: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:367:PHE:CE2	1:H:410:MET:HG3	2.38	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:D:60:GLY:HA3	1:D:423:TYR:CD2	2.38	0.58
1:E:35:LEU:HD12	1:E:436:PHE:HB2	1.85	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:A:62:ARG:HD3	4:A:2609:HOH:O	2.04	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:G:159:GLU:OE1	4:G:8505:HOH:O	2.17	0.57
1:H:134:LEU:HG	1:H:138:ARG:HD2	1.85	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:E:211:PRO:O	1:E:217:ASN:CG	2.49	0.56
1:G:78:THR:OG1	1:G:96:MET:HE1	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:HG23	1:H:19:THR:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:ARG:HB2	1:E:291:ARG:HH11	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:A:414:PRO:HD2	1:A:431:GLU:HG2	1.90	0.54
1:B:175:SER:O	1:B:176:HIS:HB2	2.07	0.54
1:A:101:PRO:HA	1:A:150:ASP:OD1	2.08	0.53
1:E:96:MET:SD	1:E:206:TYR:CE2	3.01	0.53
1:E:301:ILE:HD12	1:E:317:PHE:HB3	1.90	0.53
1:A:135:GLU:HG2	4:A:2564:HOH:O	2.07	0.53
1:C:371:CYS:HB3	1:C:409:SER:CB	2.38	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:G:247:GLN:HE21	1:G:324:PRO:HD3	1.74	0.52
1:H:371:CYS:CB	1:H:409:SER:HB2	2.40	0.52
1:E:233:LEU:HD22	1:E:238:LYS:HB2	1.91	0.52
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.74	0.52
1:F:35:LEU:HB2	1:F:135:GLU:HG3	1.92	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:G:317:PHE:HE1	1:G:319:LEU:HD21	1.74	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:222:HIS:HB3	1:E:408:THR:HG22	1.92	0.51
1:A:403:ALA:HA	1:A:408:THR:HG23	1.93	0.51
1:G:175:SER:OG	1:G:401:GLN:O	2.27	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:A:250:ASN:C	1:A:250:ASN:HD22	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:CD	1:A:342:ARG:NH1	2.69	0.51
1:H:135:GLU:HB3	1:H:436:PHE:CE1	2.46	0.51
1:A:277:MET:CE	1:A:281:MET:HE3	2.41	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:D:114:HIS:HB2	1:D:116:ASP:OD1	2.11	0.50
1:D:240:ILE:HG12	1:D:438:VAL:HG21	1.92	0.50
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:G:166:ARG:HG3	1:G:166:ARG:HH11	1.76	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:G:413:ILE:HD11	1:G:435:GLY:HA2	1.92	0.50
1:D:166:ARG:O	1:D:169:THR:HG22	2.10	0.50
1:D:238:LYS:HD2	1:D:389:ARG:HB2	1.92	0.50
1:G:171:SER:O	1:G:175:SER:HB2	2.11	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:B:92:LYS:HD2	1:B:211:PRO:HA	1.94	0.49
1:C:267:PRO:HB2	4:C:3548:HOH:O	2.11	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: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:238:LYS:HD2	1:G:389:ARG:HB2	1.94	0.49
1:B:26:ALA:HB2	1:G:291:ARG:O	2.13	0.49
1:B:169:THR:O	1:B:173:VAL:HG13	2.11	0.49
1:G:277:MET:HE2	1:G:343:LEU:HB3	1.94	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:C:378:SER:OG	1:C:441:GLN:HB3	2.11	0.49
1:E:34:ARG:CZ	1:E:138:ARG:HD2	2.42	0.49
1:A:222:HIS:O	1:A:408:THR:HB	2.13	0.48
1:E:214:TYR:HD1	1:E:214:TYR:H	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LEU:HD21	1:E:391:ILE:HD11	1.94	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:HG2	1:D:269:ARG:HH11	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:A:159:GLU:HG2	1:A:168:CYS:SG	2.54	0.47
1:F:249:TYR:CE2	1:F:362:SER:HB3	2.49	0.47
1:G:111:THR:O	1:G:153:VAL:HA	2.14	0.47
1:A:34:ARG:HG2	1:A:135:GLU:OE1	2.13	0.47
1:E:115:LEU:HD21	1:E:130:VAL:HG21	1.96	0.47
1:F:73:MET:HE2	1:F:115:LEU:HD22	1.97	0.47
1:H:57:HIS:O	1:H:123:LYS:HE2	2.15	0.47
1:A:33:GLY:O	1:A:37:GLN:HG2	2.14	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:B:287:GLU:HG3	4:B:1549:HOH:O	2.15	0.47
1:H:240:ILE:HG12	1:H:438:VAL:HG21	1.96	0.47
1:C:318:THR:C	1:C:319:LEU:HD23	2.40	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:C:414:PRO:HG2	1:C:431:GLU:CD	2.39	0.47
1:E:317:PHE:HE1	1:E:319:LEU:HD21	1.77	0.46
1:F:249:TYR:OH	1:F:360:GLN:NE2	2.47	0.46
1:G:60:GLY:HA3	1:G:423:TYR:CD2	2.50	0.46
1:H:402:THR:OG1	1:H:408:THR:HG21	2.16	0.46
1:A:18:GLY:HA2	1:A:22:LEU:HD13	1.96	0.46
1:E:30:ILE:HG21	1:E:436:PHE:CE2	2.49	0.46
1:E:78:THR:CG2	1:E:88:VAL:HG11	2.35	0.46
1:H:111:THR:O	1:H:153:VAL:HA	2.14	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:B:406:VAL:HG23	1:B:408:THR:HG22	1.97	0.46
1:F:259:VAL:HG23	1:F:272:LYS:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:THR:O	1:B:153:VAL:HA	2.17	0.45
1:B:234:GLU:OE2	1:B:417:ASP:N	2.46	0.45
1:C:100:TYR:HA	1:C:101:PRO:HD3	1.81	0.45
1:C:406:VAL:HG23	1:C:408:THR:HG22	1.97	0.45
1:E:74:ARG:HB3	1:E:206:TYR:OH	2.16	0.45
1:C:74:ARG:HB3	1:C:206:TYR:CZ	2.51	0.45
1:E:38:THR:HG21	1:E:138:ARG:HH22	1.81	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:B:292:HIS:HE1	1:B:335:GLU:OE1	2.00	0.45
1:C:171:SER:O	1:C:175:SER:HB2	2.16	0.45
1:F:36:ASN:ND2	1:F:432:ILE:HD12	2.31	0.45
1:B:96:MET:HE2	1:B:96:MET:HB3	1.77	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:A:377:ARG:HD3	1:A:377:ARG:HA	1.76	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: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:O	1:H:30:ILE:HG13	2.17	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:D:246:VAL:HG21	1:D:400:CYS:SG	2.57	0.44
1:D:157:PHE:CE1	1:D:201:LEU:HD21	2.52	0.44
1:F:45:GLN:HG2	1:F:46:PHE:CE1	2.52	0.44
1:F:128:LEU:HD21	1:F:432:ILE:HG23	1.99	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:E:245:GLY:HA2	1:E:367:PHE:CD1	2.53	0.44
1:G:310:ILE:HD12	4:G:8520:HOH:O	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:MET:CE	1:H:344:ILE:HG23	2.48	0.43
1:H:317:PHE:HE1	1:H:319:LEU:HD21	1.80	0.43
1:B:90:VAL:HG22	1:B:96:MET:HE3	1.99	0.43
1:D:111:THR:O	1:D:153:VAL:HA	2.19	0.43
1:G:323:HIS:ND1	1:G:324:PRO:HD2	2.33	0.43
1:H:107:LYS:H	1:H:107:LYS:HG3	1.55	0.43
1:C:73:MET:CE	1:C:115:LEU:HD22	2.49	0.43
1:E:99:VAL:O	1:E:99:VAL:HG12	2.18	0.43
1:H:120:GLU:HG2	1:H:423:TYR:CE2	2.54	0.43
1:B:93:ILE:O	1:B:93:ILE:HG23	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
1:A:169:THR:O	1:A:173:VAL:HG23	2.19	0.43
1:C:113:SER:HB3	1:C:130:VAL:HG23	1.99	0.43
1:D:397:HIS:CD2	1:D:410:MET:HE1	2.54	0.43
1:A:177:ASP:OD2	1:A:401:GLN:NE2	2.52	0.43
1:B:222:HIS:O	1:B:408:THR:HB	2.19	0.43
1:C:406:VAL:O	1:C:408:THR:HG23	2.19	0.43
1:E:117:THR:HB	1:E:121:ALA:CB	2.49	0.43
1:F:187:MET:HE1	1:F:196:SER:HB3	1.99	0.43
1:G:107:LYS:O	1:G:450:ARG:NH2	2.50	0.43
1:A:250:ASN:C	1:A:250:ASN:ND2	2.77	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:A:89:LYS:CD	1:A:210:THR:HG21	2.49	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: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:G:247:GLN:NE2	1:G:324:PRO:HD3	2.33	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:277:MET:HE1	1:C:343:LEU:O	2.19	0.42
1:C:344:ILE:HG23	1:C:345:LYS:HD3	1.99	0.42
1:B:168:CYS:O	1:B:172:SER:HB2	2.20	0.42
1:D:252:GLN:HB2	4:D:4554:HOH:O	2.20	0.42
1:E:124:TYR:CD2	1:E:432:ILE:HD11	2.55	0.42
1:E:271:ARG:CZ	1:E:311:ILE:HD11	2.50	0.42
1:H:371:CYS:HB2	1:H:409:SER:HB2	2.02	0.42
1:A:296:PHE:CE1	1:A:319:LEU:HD22	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:HIS:HB3	1:B:265:THR:OG1	2.19	0.42
1:A:30:ILE:HD11	1:A:440:LEU:HD22	2.01	0.42
1:C:63:ARG:HB3	1:C:117:THR:HG23	2.01	0.42
1:E:397:HIS:CD2	1:E:410:MET:HE1	2.55	0.42
1:C:362:SER:HA	1:C:363:PRO:HD3	1.79	0.42
1:F:288:ILE:HG13	1:F:291:ARG:NH2	2.34	0.42
1:F:172:SER:HA	1:F:401:GLN:HG3	2.02	0.42
1:H:378:SER:OG	1:H:441:GLN:HB3	2.19	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:C:392:TRP:HZ2	1:F:187:MET:HE3	1.85	0.41
1:C:402:THR:OG1	1:C:408:THR:HG21	2.20	0.41
1:G:298:CYS:SG	1:G:317:PHE:HB2	2.60	0.41
1:H:73:MET:HE3	1:H:115:LEU:HD22	2.01	0.41
1:B:403:ALA:HA	1:B:408:THR:HG23	2.02	0.41
1:C:290:GLN:HG2	1:D:268:TRP:CE2	2.55	0.41
1:E:127:ILE:H	1:E:127:ILE:HG12	1.53	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:D:402:THR:OG1	1:D:408:THR:HG21	2.20	0.41
1:G:339:GLU:OE2	1:G:342:ARG:NH1	2.52	0.41
1:G:398:ASP:OD1	1:G:398:ASP:N	2.44	0.41
1:H:74:ARG:HB3	1:H:206:TYR:CZ	2.56	0.41
1:H:127:ILE:H	1:H:127:ILE:HG12	1.62	0.41
1:B:319:LEU:N	1:B:319:LEU:HD23	2.36	0.41
1:C:78:THR:HB	1:C:88:VAL:HG11	2.01	0.41
1:A:22:LEU:HD11	1:A:449:TYR:HB2	2.02	0.41
1:A:111:THR:O	1:A:153:VAL:HA	2.21	0.41
1:B:242:ILE:HD12	1:B:375:VAL:HG12	2.02	0.41
1:B:443:ILE:H	1:B:443:ILE:HG12	1.71	0.41
1:D:19:THR:C	1:D:21:ASN:H	2.29	0.41
1:G:181:GLU:H	1:G:181:GLU:HG3	1.57	0.41
1:H:192:ASP:O	1:H:194:PRO:HD3	2.21	0.41
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.90	0.41
1:E:38:THR:HG21	1:E:138:ARG:NH2	2.36	0.41
1:E:224:GLU:HB3	1:E:410:MET:HG2	2.03	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:54:GLN:HE21	1:G:54:GLN:HB3	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:CE2	1:G:442:ALA:HB1	2.56	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:E:93:ILE:O	1:E:93:ILE:HG23	2.20	0.40
1:H:38:THR:O	1:H:42:THR:HG23	2.21	0.40
1:A:238:LYS:HD3	1:A:386:ASP:O	2.21	0.40
1:B:46:PHE:O	1:B:63:ARG:HD3	2.21	0.40
1:B:361:VAL:N	4:B:1525:HOH:O	2.49	0.40
1:E:38:THR:HA	1:E:41:GLU:HG2	2.02	0.40
1:E:125:ASP:O	1:E:127:ILE:HG12	2.22	0.40
1:H:77:PHE:CD2	1:H:96:MET:CE	3.04	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%)	24	48
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	24	48
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	14	35
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	24	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	24	48
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	14	35
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	43	68
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	24	48

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
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 ⓘ

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%)	322 (89%)	38 (11%)	6	17
1	B	356/383 (93%)	306 (86%)	50 (14%)	3	9
1	C	360/383 (94%)	328 (91%)	32 (9%)	9	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	360/383 (94%)	305 (85%)	55 (15%)	3	7
1	E	356/383 (93%)	272 (76%)	84 (24%)	1	2
1	F	360/383 (94%)	318 (88%)	42 (12%)	5	13
1	G	355/383 (93%)	278 (78%)	77 (22%)	1	3
1	H	360/383 (94%)	319 (89%)	41 (11%)	5	14
All	All	2867/3064 (94%)	2448 (85%)	419 (15%)	3	8

All (419) 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	78	THR
1	A	79	ASN
1	A	87	LYS
1	A	93	ILE
1	A	107	LYS
1	A	130	VAL
1	A	134	LEU
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	207	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	287	GLU
1	A	291	ARG
1	A	325	SER
1	A	334	LYS
1	A	348	ASP
1	A	361	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	GLU
1	A	384	LYS
1	A	385	LYS
1	A	387	GLN
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	96	MET
1	B	113	SER
1	B	123	LYS
1	B	127	ILE
1	B	128	LEU
1	B	134	LEU
1	B	135	GLU
1	B	139	THR
1	B	141	LYS
1	B	163	ARG
1	B	181	GLU
1	B	189	VAL
1	B	193	LYS
1	B	201	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	361	VAL
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	416	LYS
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	118	GLN
1	C	128	LEU
1	C	134	LEU
1	C	141	LYS
1	C	171	SER
1	C	197	VAL
1	C	240	ILE
1	C	252	GLN
1	C	286	SER
1	C	308	VAL
1	C	316	SER
1	C	319	LEU
1	C	325	SER
1	C	332	MET
1	C	356	SER
1	C	362	SER
1	C	408	THR
1	C	415	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	416	LYS
1	C	419	LEU
1	C	428	SER
1	C	440	LEU
1	C	443	ILE
1	C	453	ARG
1	D	20	LEU
1	D	32	SER
1	D	37	GLN
1	D	41	GLU
1	D	45	GLN
1	D	49	VAL
1	D	54	GLN
1	D	58	GLU
1	D	62	ARG
1	D	63	ARG
1	D	78	THR
1	D	87	LYS
1	D	89	LYS
1	D	93	ILE
1	D	103	LYS
1	D	107	LYS
1	D	123	LYS
1	D	127	ILE
1	D	128	LEU
1	D	141	LYS
1	D	142	ASP
1	D	146	VAL
1	D	169	THR
1	D	181	GLU
1	D	191	GLU
1	D	192	ASP
1	D	193	LYS
1	D	202	LYS
1	D	207	ILE
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	253	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	277	MET
1	D	308	VAL
1	D	310	ILE
1	D	332	MET
1	D	345	LYS
1	D	357	GLU
1	D	361	VAL
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	37	GLN
1	E	38	THR
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	63	ARG
1	E	73	MET
1	E	79	ASN
1	E	87	LYS
1	E	89	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	104	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	107	LYS
1	E	113	SER
1	E	115	LEU
1	E	127	ILE
1	E	130	VAL
1	E	131	LEU
1	E	139	THR
1	E	150	ASP
1	E	152	CYS
1	E	153	VAL
1	E	154	VAL
1	E	159	GLU
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	182	GLU
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	252	GLN
1	E	253	LYS
1	E	271	ARG
1	E	286	SER
1	E	287	GLU
1	E	291	ARG
1	E	301	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	325	SER
1	E	331	THR
1	E	334	LYS
1	E	345	LYS
1	E	356	SER
1	E	360	GLN
1	E	377	ARG
1	E	384	LYS
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
1	E	441	GLN
1	E	444	ILE
1	E	452	ILE
1	F	19	THR
1	F	30	ILE
1	F	41	GLU
1	F	49	VAL
1	F	51	ARG
1	F	54	GLN
1	F	89	LYS
1	F	93	ILE
1	F	103	LYS
1	F	107	LYS
1	F	118	GLN
1	F	123	LYS
1	F	128	LEU
1	F	134	LEU
1	F	139	THR
1	F	141	LYS
1	F	146	VAL
1	F	163	ARG
1	F	191	GLU
1	F	192	ASP
1	F	193	LYS
1	F	202	LYS
1	F	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	207	ILE
1	F	240	ILE
1	F	250	ASN
1	F	271	ARG
1	F	286	SER
1	F	288	ILE
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	433	GLU
1	F	437	LYS
1	F	455	HIS
1	G	28	LEU
1	G	30	ILE
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	88	VAL
1	G	92	LYS
1	G	93	ILE
1	G	103	LYS
1	G	107	LYS
1	G	118	GLN
1	G	128	LEU
1	G	135	GLU
1	G	139	THR
1	G	141	LYS
1	G	142	ASP
1	G	144	ASN
1	G	146	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	167	SER
1	G	175	SER
1	G	177	ASP
1	G	181	GLU
1	G	189	VAL
1	G	193	LYS
1	G	195	GLU
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	218	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	308	VAL
1	G	316	SER
1	G	322	ARG
1	G	325	SER
1	G	332	MET
1	G	334	LYS
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	385	LYS
1	G	386	ASP
1	G	387	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	40	LEU
1	H	54	GLN
1	H	73	MET
1	H	82	GLU
1	H	87	LYS
1	H	92	LYS
1	H	93	ILE
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	193	LYS
1	H	215	LYS
1	H	216	GLU
1	H	240	ILE
1	H	269	ARG
1	H	286	SER
1	H	311	ILE
1	H	322	ARG
1	H	334	LYS
1	H	344	ILE
1	H	346	ILE
1	H	355	GLU
1	H	356	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	358	THR
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	410	MET
1	H	413	ILE
1	H	433	GLU
1	H	451	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	54	GLN
1	A	158	ASN
1	A	222	HIS
1	A	247	GLN
1	A	250	ASN
1	A	309	ASN
1	A	390	GLN
1	A	401	GLN
1	A	445	ASN
1	A	455	HIS
1	B	176	HIS
1	B	247	GLN
1	B	250	ASN
1	B	252	GLN
1	B	257	HIS
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	387	GLN
1	B	401	GLN
1	B	422	ASN
1	B	434	ASN
1	B	445	ASN
1	B	448	ASN
1	C	36	ASN
1	C	57	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	79	ASN
1	C	176	HIS
1	C	247	GLN
1	C	252	GLN
1	C	293	ASN
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	257	HIS
1	D	382	GLN
1	D	387	GLN
1	D	445	ASN
1	E	36	ASN
1	E	118	GLN
1	E	229	GLN
1	E	247	GLN
1	E	250	ASN
1	E	252	GLN
1	E	434	ASN
1	F	36	ASN
1	F	54	GLN
1	F	118	GLN
1	F	250	ASN
1	F	292	HIS
1	F	293	ASN
1	F	360	GLN
1	F	387	GLN
1	F	405	HIS
1	F	434	ASN
1	F	441	GLN
1	F	455	HIS
1	G	45	GLN
1	G	54	GLN
1	G	143	ASN
1	G	247	GLN
1	G	250	ASN
1	G	382	GLN
1	G	401	GLN
1	G	405	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	45	GLN
1	H	247	GLN
1	H	250	ASN
1	H	292	HIS
1	H	360	GLN
1	H	441	GLN
1	H	448	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	5,6,6	1.00	0	5,7,7	0.80	0
3	BIB	G	8502	-	5,6,6	1.02	0	5,7,7	0.95	0
3	BIB	G	7502	-	5,6,6	0.91	0	5,7,7	0.92	0
3	BIB	B	1502	-	5,6,6	1.03	0	5,7,7	1.07	0
3	BIB	C	3502	-	5,6,6	1.02	0	5,7,7	0.97	0
3	BIB	E	6502	-	5,6,6	0.88	0	5,7,7	1.13	0
3	BIB	D	4502	-	5,6,6	0.98	0	5,7,7	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BIB	E	5502	-	5,6,6	1.02	0	5,7,7	0.73	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	-	-	0/6/6/6	-
3	BIB	G	8502	-	-	0/6/6/6	-
3	BIB	G	7502	-	-	1/6/6/6	-
3	BIB	B	1502	-	-	1/6/6/6	-
3	BIB	C	3502	-	-	1/6/6/6	-
3	BIB	E	6502	-	-	4/6/6/6	-
3	BIB	D	4502	-	-	0/6/6/6	-
3	BIB	E	5502	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1502	BIB	C5-C3-C4-N1
3	C	3502	BIB	C5-C3-C4-N1
3	G	7502	BIB	C5-C3-C4-N1
3	E	6502	BIB	C2-C3-C4-N1
3	E	6502	BIB	C2-C3-C5-O7
3	E	6502	BIB	C4-C3-C5-O7
3	E	6502	BIB	C4-C3-C5-O6

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, 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	438/462 (94%)	1.10	51 (11%) 9 8	12, 16, 19, 29	0
1	B	433/462 (93%)	0.79	33 (7%) 20 17	13, 16, 18, 20	0
1	C	438/462 (94%)	0.82	23 (5%) 32 28	13, 16, 19, 30	0
1	D	437/462 (94%)	0.67	23 (5%) 32 28	14, 16, 17, 20	0
1	E	433/462 (93%)	1.41	115 (26%) 1 1	15, 16, 17, 20	0
1	F	438/462 (94%)	0.73	20 (4%) 37 34	13, 16, 19, 31	0
1	G	430/462 (93%)	1.19	78 (18%) 3 3	13, 16, 17, 20	0
1	H	438/462 (94%)	0.87	31 (7%) 22 19	12, 16, 19, 24	0
All	All	3485/3696 (94%)	0.95	374 (10%) 11 9	12, 16, 18, 31	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	455	HIS	5.6
1	E	199	ASP	5.5
1	G	447	ASP	5.3
1	A	105	GLY	5.0
1	B	455	HIS	4.9
1	E	201	LEU	4.9
1	F	19	THR	4.8
1	H	120	GLU	4.6
1	E	211	PRO	4.6
1	B	25	ALA	4.6
1	E	176	HIS	4.6
1	H	454	GLY	4.5
1	G	394	GLY	4.4
1	A	193	LYS	4.4
1	E	221	ALA	4.4
1	G	50	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	327	ASP	4.1
1	E	183	ALA	4.1
1	F	165	ALA	4.1
1	C	19	THR	4.1
1	H	19	THR	4.0
1	E	68	ALA	4.0
1	G	443	ILE	3.9
1	E	91	ASP	3.9
1	E	93	ILE	3.9
1	C	192	ASP	3.9
1	G	55	GLU	3.8
1	E	70	ASP	3.8
1	A	216	GLU	3.8
1	F	189	VAL	3.8
1	E	197	VAL	3.8
1	H	348	ASP	3.8
1	E	194	PRO	3.7
1	G	379	ALA	3.7
1	E	312	PRO	3.7
1	E	106	GLY	3.6
1	E	212	ALA	3.6
1	G	53	GLY	3.6
1	D	20	LEU	3.5
1	H	264	GLY	3.5
1	A	455	HIS	3.5
1	G	386	ASP	3.5
1	H	87	LYS	3.5
1	A	191	GLU	3.5
1	G	312	PRO	3.4
1	E	180	LEU	3.4
1	E	151	VAL	3.4
1	E	96	MET	3.4
1	G	383	PHE	3.4
1	C	18	GLY	3.4
1	E	69	LEU	3.4
1	E	121	ALA	3.3
1	C	325	SER	3.3
1	E	219	ILE	3.3
1	E	261	ALA	3.3
1	G	370	VAL	3.3
1	E	206	TYR	3.3
1	G	436	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	86	CYS	3.2
1	E	152	CYS	3.2
1	A	20	LEU	3.2
1	A	19	THR	3.2
1	F	348	ASP	3.2
1	B	454	GLY	3.2
1	E	184	TYR	3.2
1	E	150	ASP	3.1
1	D	135	GLU	3.1
1	E	374	CYS	3.1
1	E	25	ALA	3.1
1	E	100	TYR	3.1
1	A	75	ASP	3.1
1	E	101	PRO	3.1
1	G	412	PHE	3.1
1	E	210	THR	3.1
1	H	263	ALA	3.1
1	A	199	ASP	3.1
1	G	411	ILE	3.1
1	D	146	VAL	3.1
1	E	404	PRO	3.0
1	E	204	ILE	3.0
1	G	306	TYR	3.0
1	B	105	GLY	3.0
1	G	408	THR	3.0
1	E	110	ALA	3.0
1	A	21	ASN	3.0
1	B	100	TYR	3.0
1	E	198	TYR	3.0
1	F	209	ASP	3.0
1	C	333	LEU	2.9
1	E	41	GLU	2.9
1	A	417	ASP	2.9
1	E	170	GLY	2.9
1	A	25	ALA	2.9
1	D	221	ALA	2.9
1	E	163	ARG	2.9
1	F	30	ILE	2.9
1	C	208	GLY	2.9
1	G	230	GLY	2.9
1	G	223	PHE	2.9
1	E	213	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	192	ASP	2.9
1	F	126	GLY	2.9
1	A	203	ASN	2.9
1	A	298	CYS	2.9
1	E	43	GLY	2.9
1	E	208	GLY	2.9
1	D	19	THR	2.9
1	G	26	ALA	2.9
1	F	377	ARG	2.8
1	D	142	ASP	2.8
1	G	261	ALA	2.8
1	G	388	VAL	2.8
1	A	452	ILE	2.8
1	D	192	ASP	2.8
1	F	192	ASP	2.8
1	H	86	CYS	2.8
1	H	82	GLU	2.8
1	E	76	TRP	2.8
1	A	126	GLY	2.8
1	E	185	GLY	2.8
1	F	18	GLY	2.8
1	G	112	GLY	2.8
1	G	454	GLY	2.8
1	E	92	LYS	2.8
1	D	311	ILE	2.8
1	B	136	VAL	2.8
1	C	455	HIS	2.7
1	E	182	GLU	2.7
1	G	139	THR	2.7
1	G	444	ILE	2.7
1	E	200	SER	2.7
1	A	431	GLU	2.7
1	C	216	GLU	2.7
1	G	395	ALA	2.7
1	D	50	ALA	2.7
1	D	451	VAL	2.7
1	E	164	PHE	2.7
1	G	451	VAL	2.7
1	G	301	ILE	2.7
1	D	455	HIS	2.7
1	G	323	HIS	2.7
1	D	264	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	122	GLY	2.7
1	E	205	GLY	2.7
1	E	139	THR	2.7
1	G	303	ALA	2.7
1	A	177	ASP	2.7
1	E	310	ILE	2.6
1	C	196	SER	2.6
1	E	142	ASP	2.6
1	E	207	ILE	2.6
1	H	455	HIS	2.6
1	A	432	ILE	2.6
1	B	206	TYR	2.6
1	E	149	TYR	2.6
1	E	126	GLY	2.6
1	F	454	GLY	2.6
1	E	378	SER	2.6
1	A	209	ASP	2.6
1	A	218	GLU	2.6
1	A	454	GLY	2.6
1	E	53	GLY	2.6
1	B	86	CYS	2.6
1	F	375	VAL	2.6
1	G	438	VAL	2.6
1	E	95	ASN	2.6
1	E	217	ASN	2.6
1	G	149	TYR	2.5
1	E	264	GLY	2.5
1	E	108	PRO	2.5
1	A	37	GLN	2.5
1	C	26	ALA	2.5
1	E	178	LEU	2.5
1	G	373	GLU	2.5
1	A	208	GLY	2.5
1	B	47	GLY	2.5
1	G	43	GLY	2.5
1	A	59	PHE	2.5
1	E	316	SER	2.5
1	D	66	GLY	2.5
1	E	105	GLY	2.5
1	G	414	PRO	2.5
1	A	104	ASN	2.5
1	H	331	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	113	SER	2.5
1	F	310	ILE	2.5
1	B	70	ASP	2.5
1	E	174	TRP	2.5
1	H	150	ASP	2.5
1	B	312	PRO	2.5
1	E	97	PHE	2.5
1	E	400	CYS	2.4
1	H	56	SER	2.4
1	E	405	HIS	2.4
1	E	455	HIS	2.4
1	A	68	ALA	2.4
1	B	303	ALA	2.4
1	E	98	ALA	2.4
1	A	181	GLU	2.4
1	B	369	GLU	2.4
1	D	55	GLU	2.4
1	G	433	GLU	2.4
1	F	190	GLY	2.4
1	G	241	GLY	2.4
1	E	263	ALA	2.4
1	B	311	ILE	2.4
1	E	134	LEU	2.4
1	B	209	ASP	2.4
1	A	418	GLY	2.4
1	G	33	GLY	2.4
1	E	99	VAL	2.4
1	E	74	ARG	2.4
1	H	436	PHE	2.4
1	B	276	LEU	2.4
1	E	177	ASP	2.4
1	H	116	ASP	2.4
1	E	268	TRP	2.4
1	B	264	GLY	2.4
1	H	98	ALA	2.4
1	E	67	THR	2.3
1	C	430	GLU	2.3
1	G	236	GLU	2.3
1	B	192	ASP	2.3
1	G	308	VAL	2.3
1	A	394	GLY	2.3
1	E	370	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	2.3
1	E	275	LEU	2.3
1	H	132	ALA	2.3
1	G	402	THR	2.3
1	H	265	THR	2.3
1	A	369	GLU	2.3
1	C	41	GLU	2.3
1	E	175	SER	2.3
1	H	192	ASP	2.3
1	A	299	GLY	2.3
1	B	315	VAL	2.3
1	E	115	LEU	2.3
1	E	371	CYS	2.3
1	G	152	CYS	2.3
1	E	301	ILE	2.3
1	G	111	THR	2.3
1	A	287	GLU	2.3
1	A	348	ASP	2.3
1	G	153	VAL	2.3
1	E	303	ALA	2.2
1	F	346	ILE	2.2
1	G	310	ILE	2.2
1	B	120	GLU	2.2
1	G	228	GLU	2.2
1	G	145	TYR	2.2
1	C	126	GLY	2.2
1	G	248	ALA	2.2
1	A	210	THR	2.2
1	E	402	THR	2.2
1	A	184	TYR	2.2
1	B	149	TYR	2.2
1	G	144	ASN	2.2
1	E	118	GLN	2.2
1	A	327	ASP	2.2
1	E	44	SER	2.2
1	G	122	GLY	2.2
1	G	435	GLY	2.2
1	D	276	LEU	2.2
1	E	84	LEU	2.2
1	E	225	LEU	2.2
1	G	440	LEU	2.2
1	A	207	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	227	ILE	2.2
1	G	367	PHE	2.2
1	A	165	ALA	2.2
1	G	309	ASN	2.2
1	C	299	GLY	2.2
1	G	294	GLY	2.2
1	A	188	SER	2.2
1	H	64	LEU	2.2
1	A	315	VAL	2.2
1	E	90	VAL	2.2
1	E	256	VAL	2.2
1	E	281	MET	2.2
1	A	223	PHE	2.2
1	E	39	ILE	2.2
1	G	239	ALA	2.2
1	E	224	GLU	2.2
1	C	377	ARG	2.2
1	D	312	PRO	2.2
1	E	214	TYR	2.2
1	G	101	PRO	2.2
1	H	103	LYS	2.2
1	B	43	GLY	2.2
1	F	199	ASP	2.2
1	E	311	ILE	2.2
1	E	368	HIS	2.2
1	G	30	ILE	2.2
1	G	151	VAL	2.2
1	E	46	PHE	2.2
1	G	392	TRP	2.1
1	E	138	ARG	2.1
1	D	23	PRO	2.1
1	G	104	ASN	2.1
1	G	441	GLN	2.1
1	E	48	GLY	2.1
1	B	30	ILE	2.1
1	B	154	VAL	2.1
1	E	259	VAL	2.1
1	H	344	ILE	2.1
1	B	46	PHE	2.1
1	E	321	PHE	2.1
1	G	59	PHE	2.1
1	C	165	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	GLU	2.1
1	B	194	PRO	2.1
1	E	107	LYS	2.1
1	G	390	GLN	2.1
1	G	276	LEU	2.1
1	A	435	GLY	2.1
1	G	452	ILE	2.1
1	H	257	HIS	2.1
1	E	367	PHE	2.1
1	G	113	SER	2.1
1	G	316	SER	2.1
1	A	453	ARG	2.1
1	B	266	THR	2.1
1	F	115	LEU	2.1
1	E	306	TYR	2.1
1	E	397	HIS	2.1
1	E	449	TYR	2.1
1	G	100	TYR	2.1
1	E	155	VAL	2.1
1	C	209	ASP	2.1
1	H	70	ASP	2.1
1	A	159	GLU	2.1
1	B	110	ALA	2.1
1	G	41	GLU	2.1
1	E	78	THR	2.1
1	D	440	LEU	2.1
1	E	276	LEU	2.1
1	G	233	LEU	2.1
1	B	301	ILE	2.1
1	G	249	TYR	2.1
1	H	443	ILE	2.1
1	D	315	VAL	2.1
1	A	62	ARG	2.0
1	C	417	ASP	2.0
1	D	199	ASP	2.0
1	G	380	PHE	2.1
1	B	274	ALA	2.0
1	B	430	GLU	2.0
1	C	287	GLU	2.0
1	D	41	GLU	2.0
1	G	369	GLU	2.0
1	D	193	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	169	THR	2.0
1	F	169	THR	2.0
1	E	79	ASN	2.0
1	H	104	ASN	2.0
1	H	203	ASN	2.0
1	E	102	GLY	2.0
1	E	161	GLY	2.0
1	F	161	GLY	2.0
1	H	207	ILE	2.0
1	G	328	VAL	2.0
1	H	354	TYR	2.0
1	A	317	PHE	2.0
1	G	430	GLU	2.0
1	H	357	GLU	2.0
1	E	274	ALA	2.0
1	H	336	ALA	2.0
1	G	268	TRP	2.0
1	A	64	LEU	2.0
1	B	262	HIS	2.0
1	A	411	ILE	2.0
1	C	161	GLY	2.0
1	D	301	ILE	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($\text{\AA}^2$)	Q<0.9
3	BIB	G	8502	7/7	0.62	0.17	19,21,21,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BIB	G	7502	7/7	0.66	0.18	12,13,15,15	0
3	BIB	D	4502	7/7	0.67	0.17	16,16,17,17	0
3	BIB	E	6502	7/7	0.68	0.19	21,22,24,24	0
3	BIB	E	5502	7/7	0.72	0.20	16,17,18,18	0
3	BIB	A	2502	7/7	0.75	0.17	15,19,21,21	0
3	BIB	B	1502	7/7	0.77	0.19	19,23,24,25	0
3	BIB	C	3502	7/7	0.81	0.14	24,26,27,27	0
2	ZN	E	500	1/1	0.89	0.08	16,16,16,16	0
2	ZN	E	501	1/1	0.92	0.09	18,18,18,18	0
2	ZN	G	501	1/1	0.92	0.18	17,17,17,17	0
2	ZN	F	501	1/1	0.96	0.08	18,18,18,18	0
2	ZN	D	501	1/1	0.96	0.09	18,18,18,18	0
2	ZN	B	501	1/1	0.97	0.03	18,18,18,18	0
2	ZN	D	500	1/1	0.97	0.04	15,15,15,15	0
2	ZN	A	501	1/1	0.97	0.10	18,18,18,18	0
2	ZN	H	501	1/1	0.98	0.08	18,18,18,18	0
2	ZN	G	500	1/1	0.98	0.10	15,15,15,15	0
2	ZN	B	500	1/1	0.98	0.04	16,16,16,16	0
2	ZN	C	501	1/1	0.99	0.09	18,18,18,18	0
2	ZN	C	500	1/1	0.99	0.11	16,16,16,16	0
2	ZN	H	500	1/1	0.99	0.09	15,15,15,15	0
2	ZN	F	500	1/1	1.00	0.11	16,16,16,16	0
2	ZN	A	500	1/1	1.00	0.16	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.