



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:40 AM UTC

PDB ID : 7NIT / pdb_00007nit
Title : X-ray structure of a multidomain BbgIII from Bifidobacterium bifidum
Authors : Moroz, O.V.; Blagova, E.; Lebedev, A.A.; Sanchez Rodriguez, F.; Rigden, D.J.; Tams, J.W.; Wilting, R.; Vester, J.K.; Longhin, E.; Krogh, K.B.R.; Pache, R.A.; Davies, G.J.; Wilson, K.S.
Deposited on : 2021-02-14
Resolution : 2.89 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

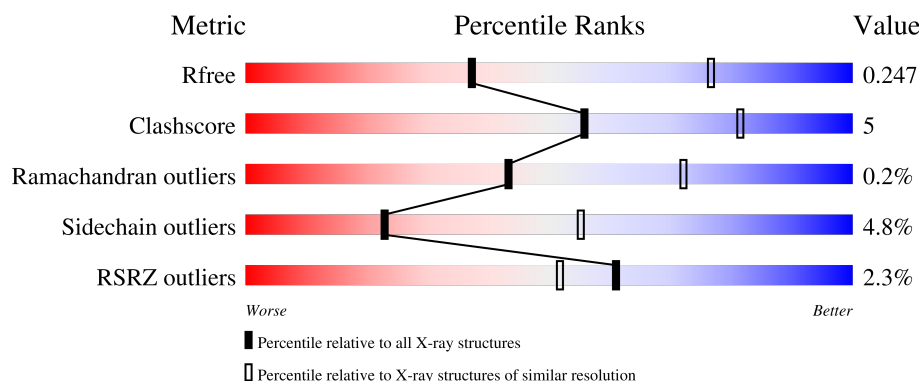
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1304	
1	B	1304	
1	C	1304	
1	D	1304	
1	E	1304	

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Mol	Chain	Length	Quality of chain
1	F	1304	

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	GOL	B	2302	-	-	X	-
3	GOL	F	2302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 55867 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1239	Total	C	N	O	S	0	0	0
			9306	5807	1585	1897	17			
1	B	1235	Total	C	N	O	S	0	0	0
			9246	5768	1574	1888	16			
1	C	1243	Total	C	N	O	S	0	0	0
			9326	5818	1585	1906	17			
1	D	1253	Total	C	N	O	S	0	0	0
			9390	5856	1601	1916	17			
1	E	1235	Total	C	N	O	S	0	0	0
			9195	5733	1567	1879	16			
1	F	1244	Total	C	N	O	S	0	0	0
			9324	5816	1586	1905	17			

There are 6 discrepancies between the modelled and reference sequences:

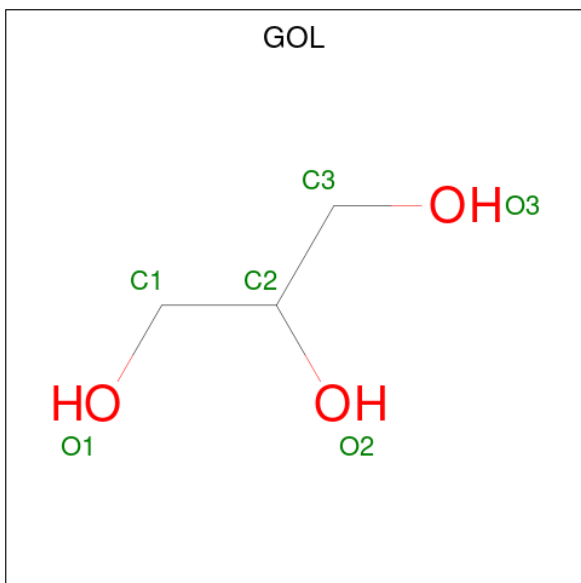
Chain	Residue	Modelled	Actual	Comment	Reference
A	1165	GLU	ASP	conflict	UNP A0A415C3Q2
B	1165	GLU	ASP	conflict	UNP A0A415C3Q2
C	1165	GLU	ASP	conflict	UNP A0A415C3Q2
D	1165	GLU	ASP	conflict	UNP A0A415C3Q2
E	1165	GLU	ASP	conflict	UNP A0A415C3Q2
F	1165	GLU	ASP	conflict	UNP A0A415C3Q2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

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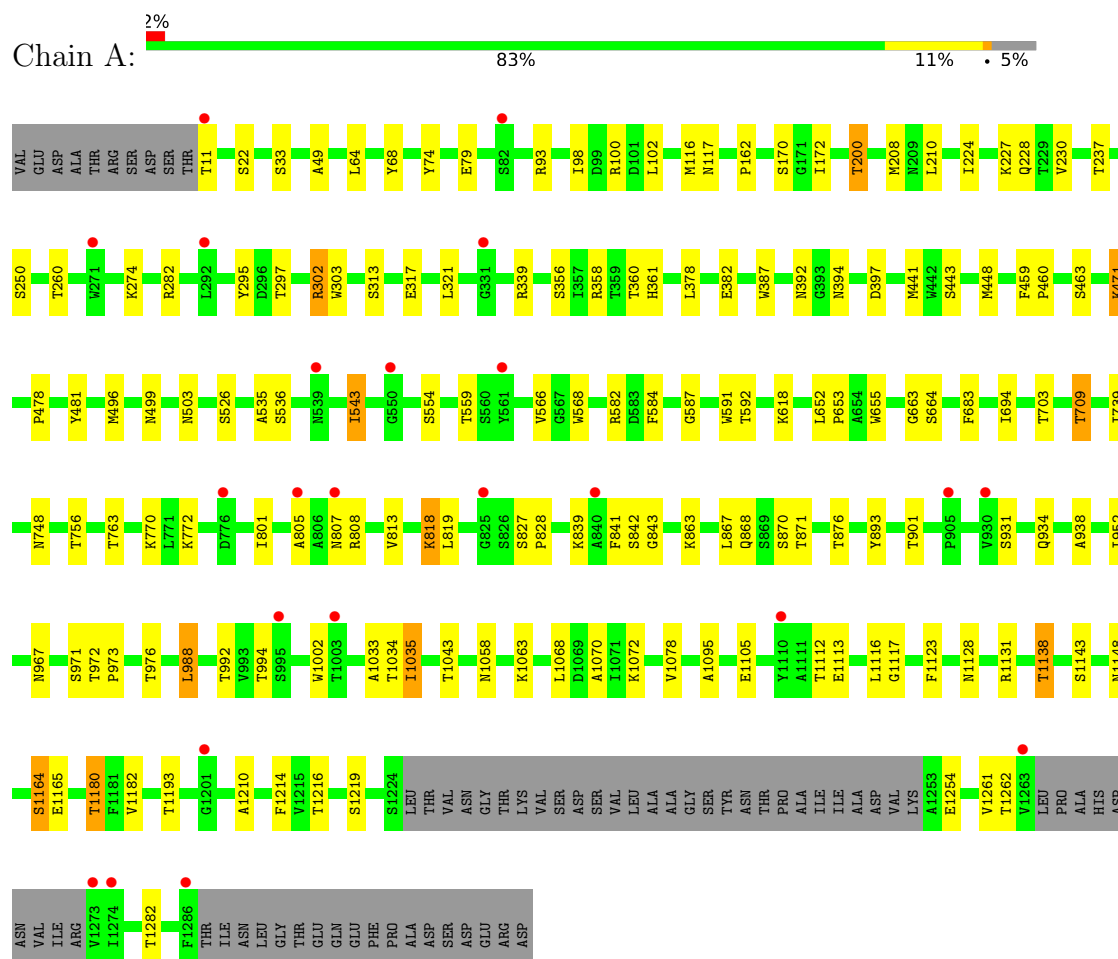
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		

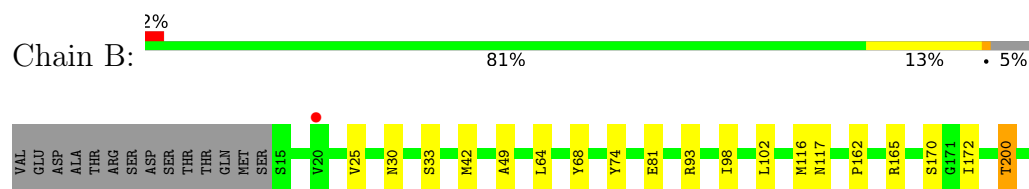
3 Residue-property plots

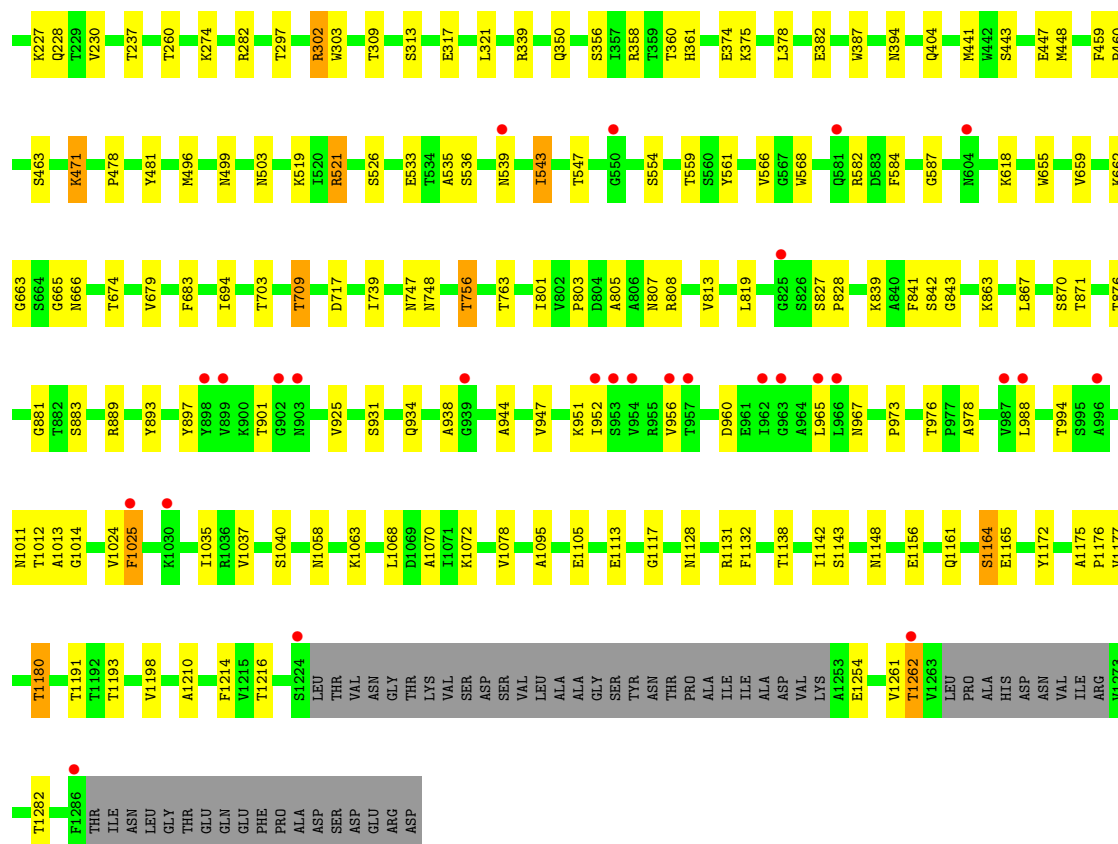
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

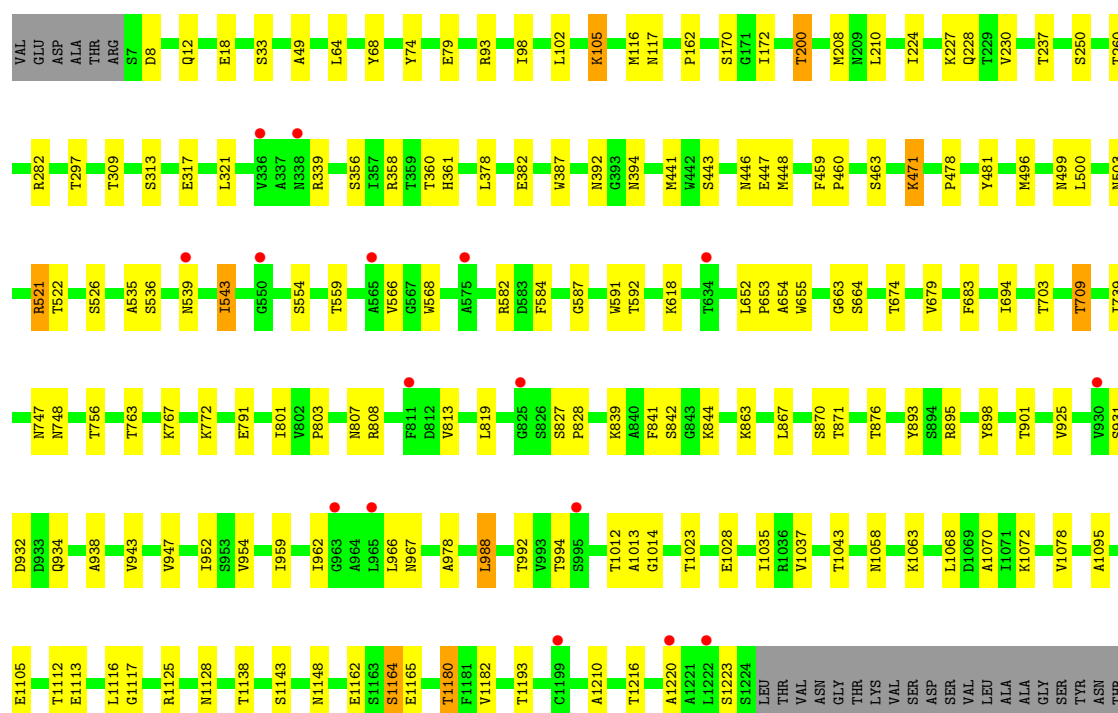
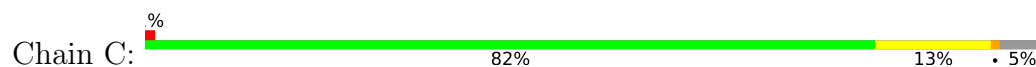


• Molecule 1: Beta-galactosidase

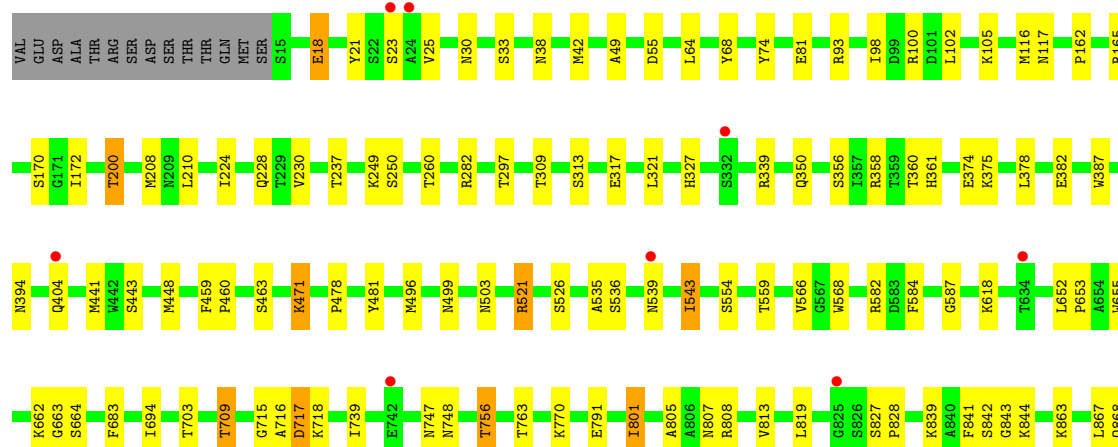
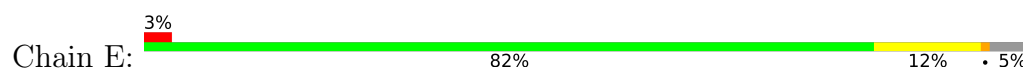


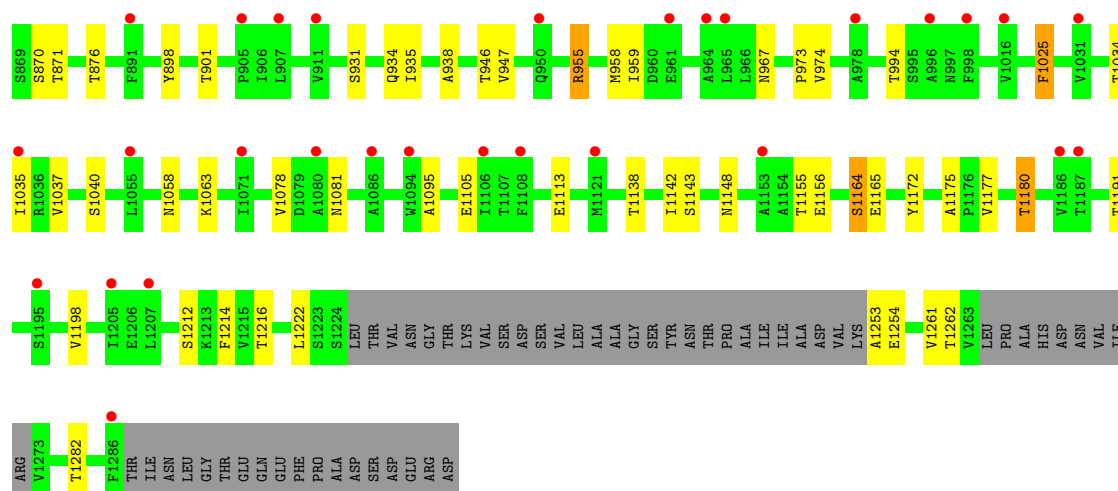


• Molecule 1: Beta-galactosidase

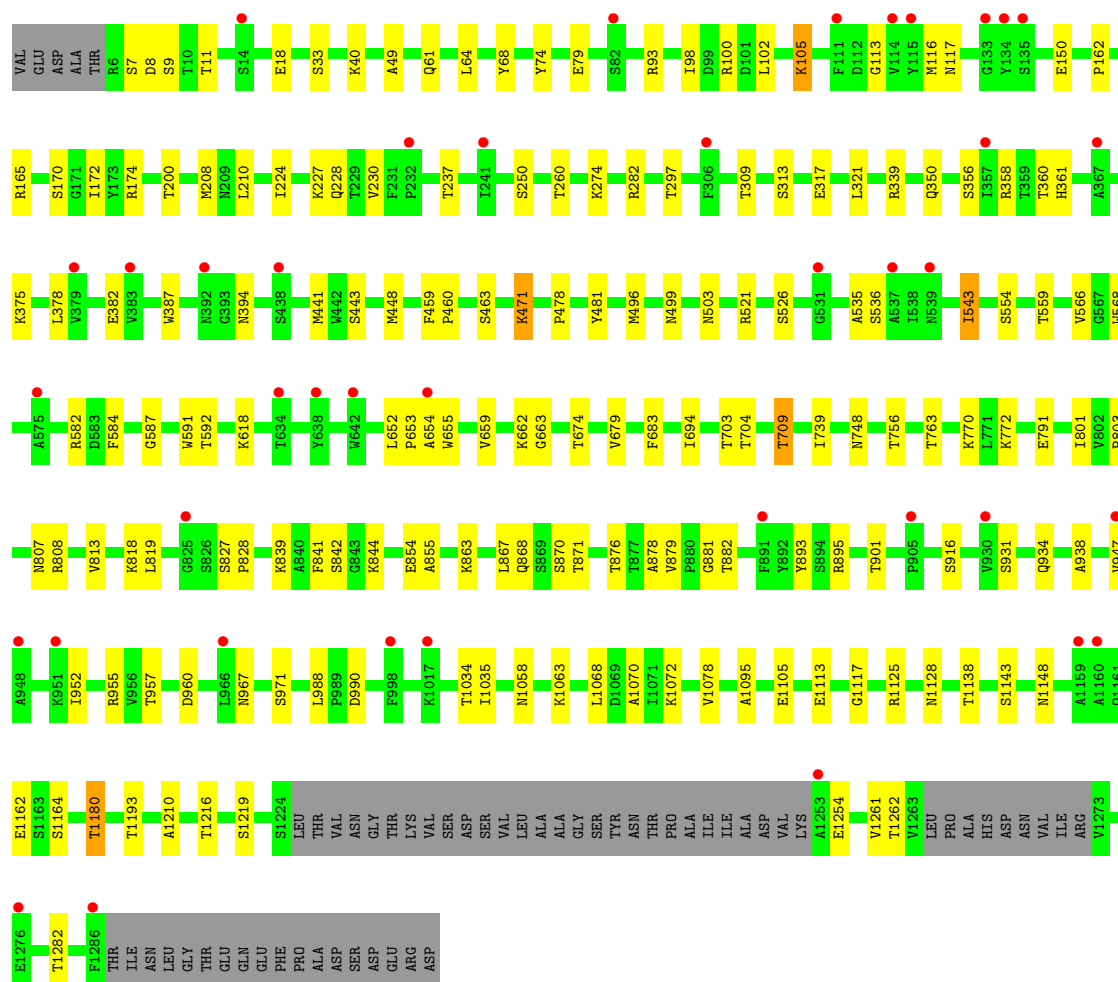
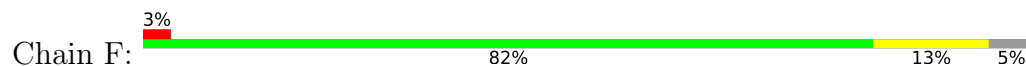


Chain D: 2% 83% 12% . .





● Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.95Å 130.04Å 200.58Å 86.99° 84.83° 83.79°	Depositor
Resolution (Å)	199.58 – 2.89 199.58 – 2.89	Depositor EDS
% Data completeness (in resolution range)	96.2 (199.58-2.89) 96.2 (199.58-2.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.247 0.214 , 0.247	Depositor DCC
R_{free} test set	12571 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55867	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, GOL

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	0.55	0/9503	1.01	3/12962 (0.0%)
1	B	0.58	0/9443	1.04	6/12889 (0.0%)
1	C	0.56	0/9523	1.01	1/12990 (0.0%)
1	D	0.56	0/9589	1.01	5/13082 (0.0%)
1	E	0.55	0/9390	1.01	6/12825 (0.0%)
1	F	0.53	0/9521	0.99	1/12990 (0.0%)
All	All	0.55	0/56969	1.01	22/77738 (0.0%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	990	ASP	CA-CB-CG	7.63	120.23	112.60
1	C	200	THR	CA-CB-OG1	-6.55	99.78	109.60
1	B	200	THR	CA-CB-OG1	-6.29	100.16	109.60
1	E	200	THR	CA-CB-OG1	-6.21	100.28	109.60
1	B	883	SER	N-CA-C	-5.78	106.00	113.16
1	E	1025	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	1025	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	200	THR	CA-CB-OG1	-5.50	101.36	109.60
1	D	763	THR	CA-CB-OG1	-5.37	101.55	109.60
1	B	519	LYS	CB-CG-CD	5.29	123.46	111.30
1	B	81	GLU	CB-CG-CD	5.25	121.53	112.60
1	D	8	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	249	LYS	CB-CG-CD	5.25	123.36	111.30
1	E	18	GLU	CB-CG-CD	5.19	121.43	112.60
1	A	11	THR	CB-CA-C	5.18	120.49	109.10
1	A	397	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	735	ALA	O-C-N	-5.14	117.62	123.48
1	E	81	GLU	CB-CG-CD	5.14	121.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	397	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	756	THR	CA-CB-OG1	-5.08	101.99	109.60
1	B	756	THR	CA-CB-OG1	-5.07	101.99	109.60
1	D	243	THR	CA-CB-OG1	-5.06	102.00	109.60

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	9306	0	8880	76	0
1	B	9246	0	8784	97	0
1	C	9326	0	8895	101	0
1	D	9390	0	8946	87	0
1	E	9195	0	8696	80	0
1	F	9324	0	8877	76	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	A	12	0	16	0	0
3	B	6	0	8	5	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
3	E	6	0	8	1	0
3	F	6	0	8	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	55867	0	53142	507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (507) 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:F:879:VAL:HB	1:F:882:THR:HG23	1.33	1.06
1:C:1023:THR:HG22	1:C:1028:GLU:HG3	1.52	0.91
1:C:959:ILE:HG21	1:C:962:ILE:HD11	1.59	0.85
1:B:1014:GLY:O	1:B:1037:VAL:HG22	1.79	0.82
1:E:1155:THR:HG22	1:F:704:THR:HA	1.65	0.79
1:C:1014:GLY:O	1:C:1037:VAL:HG22	1.83	0.79
1:D:1014:GLY:O	1:D:1037:VAL:HG22	1.81	0.79
1:C:1023:THR:CG2	1:C:1028:GLU:HG3	2.14	0.77
1:C:959:ILE:HG21	1:C:962:ILE:CD1	2.14	0.77
1:C:1012:THR:O	1:C:1037:VAL:HG21	1.89	0.73
1:D:1012:THR:O	1:D:1037:VAL:HG21	1.88	0.73
1:B:1012:THR:O	1:B:1037:VAL:HG21	1.87	0.72
1:A:988:LEU:HD11	1:A:994:THR:CG2	2.19	0.72
1:F:967:ASN:HB2	1:F:1262:THR:HG22	1.72	0.72
1:C:988:LEU:HD22	1:C:992:THR:HB	1.69	0.72
1:D:1131:ARG:HB3	1:E:747:ASN:ND2	2.05	0.71
1:E:358:ARG:HG2	1:E:360:THR:CG2	2.20	0.71
1:A:1131:ARG:HB3	1:B:747:ASN:ND2	2.05	0.71
1:A:1131:ARG:HB3	1:B:747:ASN:HD21	1.55	0.71
1:B:978:ALA:CB	1:B:1035:ILE:HD13	2.21	0.70
1:F:150:GLU:OE2	1:F:895:ARG:NH1	2.24	0.69
1:D:967:ASN:HB2	1:D:1262:THR:HG22	1.73	0.69
1:E:967:ASN:HB2	1:E:1262:THR:HG22	1.75	0.68
1:D:988:LEU:HD11	1:D:994:THR:CG2	2.24	0.68
1:C:967:ASN:HB2	1:C:1262:THR:HG22	1.76	0.68
1:F:683:PHE:HB2	1:F:694:ILE:HD11	1.76	0.68
1:A:967:ASN:HB2	1:A:1262:THR:HG22	1.74	0.67
1:E:358:ARG:HG2	1:E:360:THR:HG22	1.77	0.67
1:E:55:ASP:CG	1:E:955:ARG:NH1	2.53	0.66
1:C:162:PRO:HG2	1:C:394:ASN:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:LEU:HD12	1:D:1262:THR:HG21	1.77	0.66
1:C:8:ASP:HB2	1:C:12:GLN:O	1.96	0.65
1:C:683:PHE:HB2	1:C:694:ILE:HD11	1.76	0.65
1:A:162:PRO:HG2	1:A:394:ASN:HA	1.78	0.65
1:D:683:PHE:HB2	1:D:694:ILE:HD11	1.78	0.65
1:E:683:PHE:HB2	1:E:694:ILE:HD11	1.78	0.65
1:E:521:ARG:HG3	1:E:521:ARG:HH11	1.62	0.64
1:F:162:PRO:HG2	1:F:394:ASN:HA	1.78	0.64
1:D:1131:ARG:HB3	1:E:747:ASN:HD21	1.60	0.64
1:B:162:PRO:HG2	1:B:394:ASN:HA	1.80	0.64
1:F:591:TRP:CZ2	3:F:2302:GOL:H2	2.34	0.64
1:A:683:PHE:HB2	1:A:694:ILE:HD11	1.79	0.63
1:D:162:PRO:HG2	1:D:394:ASN:HA	1.80	0.63
1:B:521:ARG:HG3	1:B:521:ARG:HH11	1.64	0.63
1:B:988:LEU:HD11	1:B:994:THR:CG2	2.29	0.63
1:E:339:ARG:HH11	1:E:339:ARG:HG2	1.63	0.63
1:C:978:ALA:CB	1:C:1035:ILE:HD13	2.29	0.62
1:C:1125:ARG:NH1	1:C:1162:GLU:OE2	2.33	0.62
1:F:591:TRP:CH2	3:F:2302:GOL:H2	2.35	0.62
1:E:162:PRO:HG2	1:E:394:ASN:HA	1.80	0.62
1:F:591:TRP:CZ2	3:F:2302:GOL:H32	2.35	0.62
1:A:931:SER:HB3	1:A:934:GLN:HG3	1.80	0.62
1:F:8:ASP:HB3	1:F:11:THR:OG1	2.00	0.62
1:B:683:PHE:HB2	1:B:694:ILE:HD11	1.80	0.62
1:B:967:ASN:HB2	1:B:1262:THR:HG22	1.81	0.61
1:F:463:SER:HB2	1:F:496:MET:HE3	1.82	0.61
1:C:521:ARG:HG3	1:C:521:ARG:HH11	1.66	0.61
1:C:978:ALA:HB3	1:C:1035:ILE:HD13	1.83	0.61
1:B:339:ARG:HG2	1:B:339:ARG:HH11	1.66	0.61
1:D:978:ALA:CB	1:D:1035:ILE:HD13	2.30	0.61
1:B:1191:THR:O	1:B:1198:VAL:HG21	2.02	0.60
1:E:165:ARG:HH22	3:E:2302:GOL:H32	1.66	0.60
1:C:309:THR:HG23	1:C:521:ARG:NH2	2.17	0.60
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.67	0.60
1:A:463:SER:HB2	1:A:496:MET:HE3	1.84	0.60
1:D:8:ASP:HB3	1:D:11:THR:HB	1.84	0.60
1:C:463:SER:HB2	1:C:496:MET:HE3	1.83	0.60
1:E:1191:THR:O	1:E:1198:VAL:HG21	2.01	0.60
1:D:463:SER:HB2	1:D:496:MET:HE3	1.84	0.60
1:D:988:LEU:N	1:D:988:LEU:HD12	2.16	0.59
1:D:10:THR:HA	1:D:1025:PHE:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:ARG:HG3	1:D:521:ARG:HH11	1.67	0.59
1:E:387:TRP:CE2	1:E:448:MET:HG2	2.37	0.59
1:B:807:ASN:HD22	1:B:867:LEU:HD11	1.67	0.59
1:C:988:LEU:HD11	1:C:994:THR:CG2	2.33	0.59
1:E:327:HIS:CD2	1:E:360:THR:O	2.56	0.59
1:B:463:SER:HB2	1:B:496:MET:HE3	1.84	0.59
1:B:807:ASN:ND2	1:B:867:LEU:HD11	2.17	0.59
1:B:1011:ASN:HB2	1:C:522:THR:HG23	1.84	0.59
1:C:521:ARG:HH11	1:C:521:ARG:CG	2.16	0.59
1:B:931:SER:HB2	1:B:934:GLN:HG3	1.85	0.58
1:C:925:VAL:HG22	1:C:947:VAL:HG21	1.85	0.58
1:C:1220:ALA:HB3	1:C:1259:ALA:HB2	1.85	0.58
1:D:978:ALA:HB3	1:D:1035:ILE:HD13	1.84	0.58
1:E:463:SER:HB2	1:E:496:MET:HE3	1.85	0.58
1:F:931:SER:HB2	1:F:934:GLN:HG3	1.85	0.58
1:F:1125:ARG:NH1	1:F:1162:GLU:OE2	2.35	0.58
1:B:361:HIS:NE2	3:B:2302:GOL:H12	2.19	0.58
1:C:931:SER:HB2	1:C:934:GLN:HG3	1.85	0.58
1:A:988:LEU:HD11	1:A:994:THR:HG22	1.84	0.58
1:D:321:LEU:HB2	1:D:587:GLY:HA3	1.86	0.57
1:E:898:TYR:CE2	1:E:994:THR:HB	2.38	0.57
1:A:339:ARG:HG2	1:A:339:ARG:HH11	1.67	0.57
1:E:521:ARG:HH11	1:E:521:ARG:CG	2.17	0.57
1:A:807:ASN:ND2	1:A:867:LEU:HD11	2.20	0.57
1:B:988:LEU:N	1:B:988:LEU:HD12	2.20	0.57
1:D:339:ARG:HG2	1:D:339:ARG:HH11	1.69	0.57
1:E:931:SER:HB2	1:E:934:GLN:HG3	1.86	0.57
1:A:321:LEU:HB2	1:A:587:GLY:HA3	1.86	0.57
1:B:944:ALA:HB1	1:B:951:LYS:HD3	1.87	0.57
1:D:309:THR:HG23	1:D:521:ARG:NH2	2.19	0.57
1:D:931:SER:HB2	1:D:934:GLN:HG3	1.87	0.57
1:E:807:ASN:ND2	1:E:867:LEU:HD11	2.19	0.57
1:B:521:ARG:HH11	1:B:521:ARG:CG	2.17	0.57
1:F:807:ASN:ND2	1:F:867:LEU:HD11	2.20	0.57
1:D:521:ARG:HH11	1:D:521:ARG:CG	2.18	0.57
1:F:1063:LYS:O	1:F:1095:ALA:HB3	2.05	0.57
1:B:309:THR:HG23	1:B:521:ARG:NH2	2.20	0.56
1:E:55:ASP:CG	1:E:955:ARG:HH12	2.12	0.56
1:B:813:VAL:HG21	1:B:819:LEU:HB2	1.87	0.56
1:C:807:ASN:HD22	1:C:867:LEU:HD11	1.70	0.56
1:E:309:THR:HG23	1:E:521:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LYS:O	1:A:1095:ALA:HB3	2.06	0.56
1:C:807:ASN:ND2	1:C:867:LEU:HD11	2.19	0.56
1:B:1131:ARG:HB3	1:C:747:ASN:ND2	2.21	0.56
1:E:655:TRP:CZ2	1:E:739:ILE:HD11	2.40	0.56
1:F:879:VAL:HB	1:F:882:THR:CG2	2.22	0.56
1:D:807:ASN:ND2	1:D:867:LEU:HD11	2.20	0.56
1:D:655:TRP:CZ2	1:D:739:ILE:HD11	2.41	0.56
1:E:807:ASN:HD22	1:E:867:LEU:HD11	1.70	0.56
1:F:807:ASN:HD22	1:F:867:LEU:HD11	1.71	0.56
1:B:1131:ARG:HB3	1:C:747:ASN:HD21	1.70	0.55
1:B:1143:SER:HB3	1:B:1148:ASN:O	2.06	0.55
1:C:1063:LYS:O	1:C:1095:ALA:HB3	2.06	0.55
1:F:339:ARG:HG2	1:F:339:ARG:HH11	1.71	0.55
1:B:925:VAL:HG22	1:B:947:VAL:HG21	1.87	0.55
1:B:321:LEU:HB2	1:B:587:GLY:HA3	1.88	0.55
1:C:655:TRP:CZ2	1:C:739:ILE:HD11	2.41	0.55
1:D:1063:LYS:O	1:D:1095:ALA:HB3	2.06	0.55
1:E:1063:LYS:O	1:E:1095:ALA:HB3	2.06	0.55
1:C:925:VAL:HG22	1:C:947:VAL:CG2	2.37	0.55
1:C:1143:SER:HB3	1:C:1148:ASN:O	2.06	0.55
1:F:655:TRP:CZ2	1:F:739:ILE:HD11	2.42	0.55
1:B:655:TRP:CZ2	1:B:739:ILE:HD11	2.42	0.55
1:A:1143:SER:HB3	1:A:1148:ASN:O	2.07	0.54
1:E:49:ALA:O	1:E:93:ARG:NH1	2.39	0.54
1:F:1143:SER:HB3	1:F:1148:ASN:O	2.08	0.54
1:B:1063:LYS:O	1:B:1095:ALA:HB3	2.06	0.54
1:F:49:ALA:O	1:F:93:ARG:NH1	2.39	0.54
1:D:813:VAL:HG21	1:D:819:LEU:HB2	1.89	0.54
1:C:1220:ALA:HB1	1:C:1257:GLY:H	1.73	0.54
1:A:655:TRP:CZ2	1:A:739:ILE:HD11	2.42	0.54
1:A:988:LEU:CD1	1:A:994:THR:HG23	2.37	0.54
1:C:988:LEU:HD11	1:C:994:THR:HG22	1.89	0.54
1:B:447:GLU:OE1	3:B:2302:GOL:O1	2.25	0.54
1:C:321:LEU:HB2	1:C:587:GLY:HA3	1.88	0.54
1:E:321:LEU:HB2	1:E:587:GLY:HA3	1.88	0.54
1:D:1143:SER:HB3	1:D:1148:ASN:O	2.08	0.54
1:D:543:ILE:HG22	1:D:559:THR:HA	1.90	0.53
1:E:543:ILE:HG22	1:E:559:THR:HA	1.91	0.53
1:F:321:LEU:HB2	1:F:587:GLY:HA3	1.89	0.53
1:A:807:ASN:HD22	1:A:867:LEU:HD11	1.72	0.53
1:B:49:ALA:O	1:B:93:ARG:NH1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:VAL:HG22	1:B:947:VAL:CG2	2.39	0.53
1:F:18:GLU:OE2	1:F:40:LYS:NZ	2.39	0.53
1:F:309:THR:HG23	1:F:521:ARG:NH2	2.24	0.53
1:F:813:VAL:HG21	1:F:819:LEU:HB2	1.89	0.53
1:B:978:ALA:HB3	1:B:1035:ILE:HD13	1.90	0.53
1:C:49:ALA:O	1:C:93:ARG:NH1	2.40	0.53
1:B:1013:ALA:HA	1:B:1037:VAL:HG23	1.91	0.52
1:C:543:ILE:HG22	1:C:559:THR:HA	1.91	0.52
1:D:988:LEU:HD11	1:D:994:THR:HG22	1.91	0.52
1:F:350:GLN:HE22	1:F:375:LYS:HB3	1.75	0.52
1:E:1143:SER:HB3	1:E:1148:ASN:O	2.08	0.52
1:C:1013:ALA:HA	1:C:1037:VAL:HG23	1.92	0.52
1:A:543:ILE:HG22	1:A:559:THR:HA	1.92	0.52
1:D:18:GLU:OE2	1:D:40:LYS:NZ	2.40	0.52
1:F:356:SER:HA	1:F:378:LEU:O	2.10	0.52
1:A:813:VAL:HG21	1:A:819:LEU:HB2	1.91	0.51
1:F:591:TRP:CZ2	3:F:2302:GOL:C2	2.92	0.51
1:B:49:ALA:HB1	1:B:93:ARG:HD2	1.92	0.51
1:C:813:VAL:HG21	1:C:819:LEU:HB2	1.92	0.51
1:B:165:ARG:HH22	3:B:2302:GOL:C1	2.23	0.51
1:B:973:PRO:HB3	1:B:1214:PHE:CZ	2.44	0.51
1:B:1025:PHE:HD1	1:B:1025:PHE:O	1.93	0.51
1:D:295:TYR:CE2	1:D:297:THR:HG23	2.46	0.51
1:D:807:ASN:HD22	1:D:867:LEU:HD11	1.74	0.51
1:E:49:ALA:HB1	1:E:93:ARG:HD2	1.92	0.51
1:F:543:ILE:HG22	1:F:559:THR:HA	1.92	0.51
1:A:988:LEU:HD12	1:A:988:LEU:N	2.27	0.50
1:B:543:ILE:HG22	1:B:559:THR:HA	1.92	0.50
1:B:566:VAL:HG21	1:B:568:TRP:CE2	2.46	0.50
1:A:49:ALA:O	1:A:93:ARG:NH1	2.41	0.50
1:E:350:GLN:HE22	1:E:375:LYS:HB3	1.76	0.50
1:D:49:ALA:O	1:D:93:ARG:NH1	2.40	0.50
1:E:813:VAL:HG21	1:E:819:LEU:HB2	1.93	0.50
1:A:295:TYR:CE2	1:A:297:THR:HG23	2.46	0.50
1:B:356:SER:HA	1:B:378:LEU:O	2.12	0.50
1:C:703:THR:OG1	1:C:709:THR:HB	2.12	0.50
1:C:1058:ASN:HB2	1:C:1105:GLU:H	1.77	0.50
1:D:49:ALA:HB1	1:D:93:ARG:HD2	1.94	0.50
1:D:356:SER:HA	1:D:378:LEU:O	2.12	0.50
1:A:566:VAL:HG21	1:A:568:TRP:CE2	2.46	0.50
1:E:973:PRO:HB3	1:E:1214:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:HA	1:A:378:LEU:O	2.12	0.49
1:B:1156:GLU:HG3	1:B:1172:TYR:CE2	2.47	0.49
1:F:566:VAL:HG21	1:F:568:TRP:CE2	2.47	0.49
1:C:988:LEU:HD13	1:C:992:THR:O	2.13	0.49
1:B:1058:ASN:HB2	1:B:1105:GLU:H	1.77	0.49
1:C:566:VAL:HG21	1:C:568:TRP:CE2	2.47	0.49
1:F:703:THR:OG1	1:F:709:THR:HB	2.13	0.49
1:C:356:SER:HA	1:C:378:LEU:O	2.12	0.49
1:D:566:VAL:HG21	1:D:568:TRP:CE2	2.47	0.49
1:E:356:SER:HA	1:E:378:LEU:O	2.12	0.49
1:C:901:THR:HG21	1:C:938:ALA:HB2	1.94	0.49
1:B:925:VAL:HG13	1:B:947:VAL:HG23	1.93	0.49
1:A:703:THR:OG1	1:A:709:THR:HB	2.13	0.48
1:D:1013:ALA:HA	1:D:1037:VAL:HG23	1.93	0.48
1:E:441:MET:HG2	1:E:478:PRO:HG2	1.96	0.48
1:A:901:THR:HG21	1:A:938:ALA:HB2	1.96	0.48
1:A:1117:GLY:HA3	1:A:1210:ALA:HB2	1.96	0.48
1:E:1156:GLU:HG3	1:E:1172:TYR:CE2	2.48	0.48
1:C:1014:GLY:N	1:C:1037:VAL:HG23	2.28	0.48
1:D:1266:ALA:O	1:D:1267:HIS:CB	2.61	0.48
1:D:703:THR:OG1	1:D:709:THR:HB	2.13	0.48
1:E:448:MET:HB2	1:E:448:MET:HE2	1.60	0.48
1:E:566:VAL:HG21	1:E:568:TRP:CE2	2.48	0.48
1:C:441:MET:HG2	1:C:478:PRO:HG2	1.95	0.48
1:E:360:THR:HA	1:E:361:HIS:HA	1.72	0.48
1:E:703:THR:OG1	1:E:709:THR:HB	2.13	0.48
1:D:1113:GLU:HB2	1:D:1180:THR:HG22	1.94	0.48
1:E:360:THR:HB	1:E:361:HIS:CE1	2.49	0.48
1:C:988:LEU:CD1	1:C:994:THR:HG23	2.44	0.48
1:C:1223:SER:OG	1:C:1254:GLU:O	2.27	0.48
1:D:988:LEU:CD1	1:D:994:THR:HG23	2.44	0.48
1:B:441:MET:HG2	1:B:478:PRO:HG2	1.95	0.48
1:E:1025:PHE:O	1:E:1025:PHE:HD1	1.97	0.47
1:C:1023:THR:HG22	1:C:1028:GLU:CG	2.36	0.47
1:D:901:THR:HG21	1:D:938:ALA:HB2	1.96	0.47
1:E:827:SER:N	1:E:828:PRO:CD	2.78	0.47
1:A:827:SER:N	1:A:828:PRO:CD	2.78	0.47
1:B:827:SER:N	1:B:828:PRO:CD	2.77	0.47
1:B:1117:GLY:HA3	1:B:1210:ALA:HB2	1.97	0.47
1:D:827:SER:N	1:D:828:PRO:CD	2.77	0.47
1:A:1058:ASN:HB2	1:A:1105:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HB1	1:C:93:ARG:HD2	1.97	0.47
1:B:703:THR:OG1	1:B:709:THR:HB	2.14	0.47
1:D:471:LYS:HE3	1:D:503:ASN:HB3	1.97	0.47
1:C:925:VAL:HG13	1:C:947:VAL:HG23	1.97	0.47
1:C:943:VAL:HB	1:C:954:VAL:CG2	2.45	0.47
1:D:1014:GLY:N	1:D:1037:VAL:HG23	2.30	0.47
1:E:715:GLY:O	1:E:718:LYS:HB3	2.14	0.47
1:F:49:ALA:HB1	1:F:93:ARG:HD2	1.95	0.47
1:A:49:ALA:HB1	1:A:93:ARG:HD2	1.95	0.47
1:B:64:LEU:HD13	1:B:172:ILE:HG21	1.97	0.47
1:C:827:SER:N	1:C:828:PRO:CD	2.78	0.47
1:D:441:MET:HG2	1:D:478:PRO:HG2	1.97	0.47
1:B:988:LEU:CD1	1:B:994:THR:HG23	2.45	0.47
1:A:64:LEU:HD13	1:A:172:ILE:HG21	1.98	0.46
1:E:1113:GLU:HB2	1:E:1180:THR:HG22	1.97	0.46
1:D:1113:GLU:CB	1:D:1180:THR:HG22	2.46	0.46
1:F:827:SER:N	1:F:828:PRO:CD	2.78	0.46
1:C:1023:THR:CG2	1:C:1028:GLU:CG	2.91	0.46
1:D:1058:ASN:HB2	1:D:1105:GLU:H	1.80	0.46
1:A:74:TYR:CE1	1:A:618:LYS:HG3	2.50	0.46
1:B:951:LYS:HD2	1:B:952:ILE:O	2.16	0.46
1:A:931:SER:HB3	1:A:934:GLN:CG	2.46	0.46
1:A:988:LEU:CD1	1:A:988:LEU:N	2.79	0.46
1:D:210:LEU:HD12	1:D:210:LEU:N	2.30	0.46
1:D:966:LEU:CD1	1:D:1262:THR:HG21	2.44	0.46
1:F:64:LEU:HD13	1:F:172:ILE:HG21	1.97	0.46
1:F:1113:GLU:HB2	1:F:1180:THR:HG22	1.98	0.46
1:B:1014:GLY:N	1:B:1037:VAL:HG23	2.31	0.46
1:F:1058:ASN:HB2	1:F:1105:GLU:H	1.81	0.46
1:C:988:LEU:CD1	1:C:988:LEU:N	2.78	0.46
1:D:74:TYR:CE1	1:D:618:LYS:HG3	2.51	0.46
1:F:165:ARG:HH22	3:F:2302:GOL:H11	1.80	0.46
1:C:1014:GLY:H	1:C:1037:VAL:HG23	1.81	0.46
1:E:716:ALA:C	1:E:718:LYS:H	2.23	0.45
1:F:901:THR:HG21	1:F:938:ALA:HB2	1.97	0.45
1:D:358:ARG:HG2	1:D:360:THR:HG23	1.97	0.45
1:D:988:LEU:N	1:D:988:LEU:CD1	2.79	0.45
1:E:64:LEU:HD13	1:E:172:ILE:HG21	1.98	0.45
1:F:361:HIS:CD2	3:F:2302:GOL:HO2	2.33	0.45
1:A:441:MET:HG2	1:A:478:PRO:HG2	1.98	0.45
1:B:208:MET:SD	1:B:230:VAL:HG21	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:HD13	1:D:172:ILE:HG21	1.98	0.45
1:E:360:THR:HB	1:E:361:HIS:ND1	2.32	0.45
1:E:1254:GLU:HA	1:E:1261:VAL:HG21	1.98	0.45
1:A:210:LEU:N	1:A:210:LEU:HD12	2.32	0.45
1:A:1113:GLU:HB2	1:A:1180:THR:HG22	1.99	0.45
1:E:901:THR:HG21	1:E:938:ALA:HB2	1.99	0.45
1:A:988:LEU:CD1	1:A:994:THR:CG2	2.91	0.45
1:A:1254:GLU:HA	1:A:1261:VAL:HG21	1.97	0.45
1:C:210:LEU:N	1:C:210:LEU:HD12	2.32	0.45
1:A:818:LYS:HE2	1:A:818:LYS:HB3	1.81	0.45
1:B:582:ARG:HB3	1:B:584:PHE:CE1	2.52	0.45
1:B:973:PRO:HG2	1:B:976:THR:HB	1.98	0.45
1:D:1117:GLY:HA3	1:D:1210:ALA:HB2	1.98	0.45
1:F:74:TYR:CE1	1:F:618:LYS:HG3	2.52	0.45
1:A:228:GLN:HA	1:A:282:ARG:O	2.17	0.45
1:B:665:GLY:O	1:B:666:ASN:HB2	2.16	0.45
1:F:854:GLU:OE2	1:F:916:SER:HA	2.16	0.45
1:F:1113:GLU:CB	1:F:1180:THR:HG22	2.47	0.45
1:B:965:LEU:HD21	1:B:1024:VAL:HG21	1.99	0.45
1:C:228:GLN:HA	1:C:282:ARG:O	2.16	0.45
1:D:459:PHE:N	1:D:460:PRO:HD2	2.32	0.45
1:E:791:GLU:OE2	1:E:844:LYS:HE2	2.17	0.45
1:E:1113:GLU:CB	1:E:1180:THR:HG22	2.47	0.45
1:F:591:TRP:CH2	3:F:2302:GOL:C2	2.99	0.45
1:C:988:LEU:N	1:C:988:LEU:HD12	2.31	0.45
1:D:392:ASN:OD1	1:D:1112:THR:HG21	2.17	0.45
1:D:988:LEU:CD1	1:D:988:LEU:H	2.30	0.45
1:C:392:ASN:OD1	1:C:1112:THR:HG21	2.17	0.44
1:D:228:GLN:HA	1:D:282:ARG:O	2.17	0.44
1:E:98:ILE:HG23	1:E:102:LEU:HD12	1.99	0.44
1:F:105:LYS:HA	1:F:105:LYS:HD3	1.90	0.44
1:A:302:ARG:HG2	1:A:303:TRP:N	2.33	0.44
1:B:1175:ALA:O	1:B:1177:VAL:HG23	2.17	0.44
1:F:228:GLN:HA	1:F:282:ARG:O	2.17	0.44
1:C:74:TYR:CE1	1:C:618:LYS:HG3	2.52	0.44
1:D:1254:GLU:HA	1:D:1261:VAL:HG21	1.99	0.44
1:B:228:GLN:HA	1:B:282:ARG:O	2.17	0.44
1:C:966:LEU:HD12	1:C:1262:THR:HG21	1.99	0.44
1:D:100:ARG:HG2	1:D:148:GLY:HA3	2.00	0.44
1:D:988:LEU:HD11	1:D:994:THR:HG23	1.99	0.44
1:F:674:THR:HG21	1:F:679:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:GLU:CB	1:A:1180:THR:HG22	2.47	0.44
1:B:116:MET:HE2	1:B:117:ASN:OD1	2.18	0.44
1:D:893:TYR:OH	1:D:952:ILE:HG23	2.18	0.44
1:F:441:MET:HG2	1:F:478:PRO:HG2	1.99	0.44
1:F:893:TYR:OH	1:F:952:ILE:HG23	2.17	0.44
1:A:841:PHE:O	1:A:842:SER:C	2.61	0.44
1:C:471:LYS:HE3	1:C:503:ASN:HB3	2.00	0.44
1:E:74:TYR:CE1	1:E:618:LYS:HG3	2.53	0.44
1:F:855:ALA:HB2	1:F:878:ALA:HB2	1.99	0.44
1:A:387:TRP:CE2	1:A:448:MET:HG2	2.52	0.44
1:A:1131:ARG:HD2	1:B:747:ASN:ND2	2.33	0.44
1:B:74:TYR:CE1	1:B:618:LYS:HG3	2.52	0.44
1:B:808:ARG:HA	1:B:839:LYS:HA	2.00	0.44
1:C:591:TRP:HA	1:C:592:THR:HA	1.78	0.44
1:C:1117:GLY:HA3	1:C:1210:ALA:HB2	1.99	0.44
1:E:582:ARG:HB3	1:E:584:PHE:CE1	2.53	0.44
1:C:1223:SER:HG	1:C:1254:GLU:C	2.23	0.44
1:E:228:GLN:HA	1:E:282:ARG:O	2.18	0.44
1:B:521:ARG:CG	1:B:521:ARG:NH1	2.81	0.44
1:B:841:PHE:O	1:B:842:SER:C	2.61	0.44
1:D:116:MET:HE2	1:D:117:ASN:OD1	2.18	0.44
1:A:116:MET:HE2	1:A:117:ASN:OD1	2.18	0.43
1:A:808:ARG:HA	1:A:839:LYS:HA	2.00	0.43
1:B:1113:GLU:CB	1:B:1180:THR:HG22	2.48	0.43
1:D:360:THR:HA	1:D:361:HIS:HA	1.77	0.43
1:B:358:ARG:HG2	1:B:360:THR:HG23	2.00	0.43
1:C:1113:GLU:CB	1:C:1180:THR:HG22	2.48	0.43
1:F:459:PHE:N	1:F:460:PRO:HD2	2.33	0.43
1:F:841:PHE:O	1:F:842:SER:C	2.62	0.43
1:B:165:ARG:HH22	3:B:2302:GOL:H12	1.82	0.43
1:B:210:LEU:HD12	1:B:210:LEU:N	2.33	0.43
1:B:350:GLN:HE22	1:B:375:LYS:HB3	1.83	0.43
1:D:973:PRO:HB3	1:D:1214:PHE:CZ	2.53	0.43
1:E:459:PHE:N	1:E:460:PRO:HD2	2.33	0.43
1:E:1222:LEU:HD22	1:E:1253:ALA:HB1	2.01	0.43
1:A:988:LEU:HD22	1:A:992:THR:HB	2.00	0.43
1:B:382:GLU:HA	1:B:443:SER:HB3	2.00	0.43
1:C:959:ILE:HG21	1:C:962:ILE:HD13	1.98	0.43
1:A:387:TRP:CZ2	1:A:448:MET:HG2	2.53	0.43
1:C:358:ARG:HG2	1:C:360:THR:HG23	2.00	0.43
1:C:360:THR:HA	1:C:361:HIS:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:805:ALA:HB3	1:D:843:GLY:HA2	2.00	0.43
1:B:901:THR:HG21	1:B:938:ALA:HB2	2.00	0.43
1:C:98:ILE:HG23	1:C:102:LEU:HD12	2.00	0.43
1:C:841:PHE:O	1:C:842:SER:C	2.62	0.43
1:D:582:ARG:HB3	1:D:584:PHE:CE1	2.54	0.43
1:D:713:TYR:OH	1:D:717:ASP:OD1	2.21	0.43
1:D:973:PRO:HG2	1:D:976:THR:HB	2.00	0.43
1:E:382:GLU:HA	1:E:443:SER:HB3	2.01	0.43
1:F:360:THR:HA	1:F:361:HIS:HA	1.79	0.43
1:A:471:LYS:HE3	1:A:503:ASN:HB3	2.00	0.43
1:A:805:ALA:HB3	1:A:843:GLY:HA2	2.01	0.43
1:B:98:ILE:HG23	1:B:102:LEU:HD12	2.01	0.43
1:D:382:GLU:HA	1:D:443:SER:HB3	2.01	0.43
1:F:591:TRP:CZ2	3:F:2302:GOL:C3	3.00	0.43
1:E:808:ARG:HA	1:E:839:LYS:HA	1.99	0.43
1:F:654:ALA:HB1	1:F:803:PRO:HG3	2.00	0.43
1:F:879:VAL:HG12	1:F:881:GLY:H	1.84	0.43
1:B:893:TYR:OH	1:B:952:ILE:HG23	2.18	0.43
1:E:471:LYS:HE3	1:E:503:ASN:HB3	2.01	0.43
1:F:387:TRP:CZ2	1:F:448:MET:HG2	2.54	0.43
1:A:358:ARG:HG2	1:A:360:THR:HG23	2.00	0.42
1:A:1068:LEU:C	1:A:1070:ALA:H	2.27	0.42
1:B:302:ARG:HG2	1:B:303:TRP:N	2.34	0.42
1:C:64:LEU:HD13	1:C:172:ILE:HG21	2.00	0.42
1:D:535:ALA:O	1:D:536:SER:OG	2.29	0.42
1:D:841:PHE:O	1:D:842:SER:C	2.61	0.42
1:E:1175:ALA:O	1:E:1177:VAL:HG23	2.18	0.42
1:F:382:GLU:HA	1:F:443:SER:HB3	2.01	0.42
1:B:459:PHE:N	1:B:460:PRO:HD2	2.34	0.42
1:C:459:PHE:N	1:C:460:PRO:HD2	2.35	0.42
1:D:302:ARG:HG2	1:D:303:TRP:N	2.33	0.42
1:F:791:GLU:OE2	1:F:844:LYS:HE2	2.18	0.42
1:A:1116:LEU:HD11	1:A:1182:VAL:HG21	2.02	0.42
1:C:105:LYS:HA	1:C:105:LYS:HD3	1.90	0.42
1:C:582:ARG:HB3	1:C:584:PHE:CE1	2.55	0.42
1:F:210:LEU:N	1:F:210:LEU:HD12	2.34	0.42
1:A:893:TYR:OH	1:A:952:ILE:HG23	2.19	0.42
1:D:387:TRP:CE2	1:D:448:MET:HG2	2.54	0.42
1:E:25:VAL:HG12	1:E:102:LEU:HD11	2.02	0.42
1:F:98:ILE:HG23	1:F:102:LEU:HD12	2.00	0.42
1:F:770:LYS:HD3	1:F:868:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LYS:HD3	1:A:868:GLN:OE1	2.20	0.42
1:A:973:PRO:HG2	1:A:976:THR:HB	2.02	0.42
1:A:988:LEU:HD13	1:A:992:THR:O	2.20	0.42
1:B:897:TYR:O	1:B:956:VAL:HA	2.20	0.42
1:D:808:ARG:HA	1:D:839:LYS:HA	2.00	0.42
1:E:1058:ASN:HB2	1:E:1105:GLU:H	1.85	0.42
1:A:459:PHE:N	1:A:460:PRO:HD2	2.34	0.42
1:A:582:ARG:HB3	1:A:584:PHE:CE1	2.55	0.42
1:C:1113:GLU:HB2	1:C:1180:THR:HG22	2.01	0.42
1:D:387:TRP:CZ2	1:D:448:MET:HG2	2.54	0.42
1:D:674:THR:HG21	1:D:679:VAL:HG21	2.01	0.42
1:E:770:LYS:HD3	1:E:868:GLN:OE1	2.20	0.42
1:E:805:ALA:HB3	1:E:843:GLY:HA2	2.01	0.42
1:F:808:ARG:HA	1:F:839:LYS:HA	2.02	0.42
1:D:68:TYR:CZ	1:D:170:SER:HB3	2.54	0.42
1:E:68:TYR:CZ	1:E:170:SER:HB3	2.55	0.42
1:E:116:MET:HE2	1:E:117:ASN:OD1	2.20	0.42
1:E:652:LEU:HB2	1:E:653:PRO:HA	2.01	0.42
1:C:116:MET:HE2	1:C:117:ASN:OD1	2.19	0.42
1:A:382:GLU:HA	1:A:443:SER:HB3	2.01	0.42
1:B:387:TRP:CZ2	1:B:448:MET:HG2	2.54	0.42
1:B:659:VAL:HG11	1:B:803:PRO:HB2	2.00	0.42
1:B:1132:PHE:HB2	1:C:747:ASN:OD1	2.19	0.42
1:E:358:ARG:HG2	1:E:360:THR:HG23	1.98	0.42
1:E:801:ILE:H	1:E:801:ILE:HG12	1.63	0.42
1:E:935:ILE:HA	1:E:958:MET:HE3	2.02	0.42
1:E:974:VAL:HG22	1:E:1037:VAL:HG12	2.02	0.42
1:F:659:VAL:HG11	1:F:803:PRO:HB2	2.01	0.42
1:F:1254:GLU:HA	1:F:1261:VAL:HG21	2.02	0.42
1:A:98:ILE:HG23	1:A:102:LEU:HD12	2.00	0.42
1:A:208:MET:SD	1:A:230:VAL:HG21	2.60	0.42
1:B:533:GLU:OE2	3:B:2302:GOL:O1	2.31	0.42
1:B:988:LEU:CD1	1:B:994:THR:CG2	2.97	0.42
1:C:1068:LEU:C	1:C:1070:ALA:H	2.27	0.42
1:A:591:TRP:HA	1:A:592:THR:HA	1.78	0.41
1:C:208:MET:SD	1:C:230:VAL:HG21	2.60	0.41
1:C:500:LEU:HD23	1:C:500:LEU:HA	1.94	0.41
1:C:988:LEU:CD1	1:C:994:THR:CG2	2.98	0.41
1:F:1068:LEU:C	1:F:1070:ALA:H	2.28	0.41
1:B:25:VAL:HG12	1:B:102:LEU:HD11	2.02	0.41
1:B:471:LYS:HE3	1:B:503:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:GLU:HB2	1:B:1180:THR:HG22	2.01	0.41
1:C:68:TYR:CZ	1:C:170:SER:HB3	2.55	0.41
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.80	0.41
1:C:791:GLU:OE2	1:C:844:LYS:HE2	2.20	0.41
1:D:935:ILE:HA	1:D:958:MET:HE3	2.03	0.41
1:E:208:MET:SD	1:E:230:VAL:HG21	2.60	0.41
1:E:717:ASP:OD1	1:E:717:ASP:N	2.48	0.41
1:A:392:ASN:OD1	1:A:1112:THR:HG21	2.21	0.41
1:B:387:TRP:CE2	1:B:448:MET:HG2	2.56	0.41
1:C:446:ASN:O	1:C:447:GLU:C	2.63	0.41
1:C:1128:ASN:O	1:C:1193:THR:HB	2.20	0.41
1:F:116:MET:HE2	1:F:117:ASN:OD1	2.20	0.41
1:F:358:ARG:HG2	1:F:360:THR:HG23	2.01	0.41
1:D:521:ARG:CG	1:D:521:ARG:NH1	2.82	0.41
1:F:652:LEU:HB2	1:F:653:PRO:HA	2.02	0.41
1:A:68:TYR:CZ	1:A:170:SER:HB3	2.55	0.41
1:C:663:GLY:O	1:C:664:SER:C	2.63	0.41
1:C:988:LEU:CD1	1:C:988:LEU:H	2.34	0.41
1:D:25:VAL:HG12	1:D:102:LEU:HD11	2.02	0.41
1:D:988:LEU:HD12	1:D:988:LEU:H	1.84	0.41
1:A:663:GLY:O	1:A:664:SER:C	2.63	0.41
1:C:652:LEU:HB2	1:C:653:PRO:HA	2.02	0.41
1:C:1116:LEU:HD11	1:C:1182:VAL:HG21	2.01	0.41
1:E:1040:SER:HB3	1:E:1212:SER:HB3	2.02	0.41
1:F:208:MET:SD	1:F:230:VAL:HG21	2.61	0.41
1:A:973:PRO:HB3	1:A:1214:PHE:CZ	2.56	0.41
1:B:717:ASP:OD1	1:B:717:ASP:N	2.48	0.41
1:B:805:ALA:HB3	1:B:843:GLY:HA2	2.01	0.41
1:B:1254:GLU:HA	1:B:1261:VAL:HG21	2.03	0.41
1:C:808:ARG:HA	1:C:839:LYS:HA	2.01	0.41
1:B:68:TYR:CZ	1:B:170:SER:HB3	2.56	0.41
1:D:98:ILE:HG23	1:D:102:LEU:HD12	2.03	0.41
1:D:1014:GLY:H	1:D:1037:VAL:HG23	1.83	0.41
1:F:68:TYR:CZ	1:F:170:SER:HB3	2.56	0.41
1:A:652:LEU:HB2	1:A:653:PRO:HA	2.03	0.41
1:A:1164:SER:O	1:A:1165:GLU:C	2.64	0.41
1:B:1128:ASN:O	1:B:1193:THR:HB	2.21	0.41
1:C:382:GLU:HA	1:C:443:SER:HB3	2.02	0.41
1:D:1068:LEU:C	1:D:1070:ALA:H	2.27	0.41
1:E:210:LEU:N	1:E:210:LEU:HD12	2.35	0.41
1:E:841:PHE:O	1:E:842:SER:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1164:SER:O	1:E:1165:GLU:C	2.64	0.41
1:F:1117:GLY:HA3	1:F:1210:ALA:HB2	2.02	0.41
1:F:1128:ASN:O	1:F:1193:THR:HB	2.21	0.41
1:A:360:THR:HA	1:A:361:HIS:HA	1.76	0.41
1:C:654:ALA:HB1	1:C:803:PRO:HG3	2.03	0.41
1:F:471:LYS:HE3	1:F:503:ASN:HB3	2.03	0.41
1:F:582:ARG:HB3	1:F:584:PHE:CE1	2.55	0.41
1:B:1068:LEU:C	1:B:1070:ALA:H	2.29	0.40
1:C:674:THR:HG21	1:C:679:VAL:HG21	2.02	0.40
1:D:1128:ASN:O	1:D:1193:THR:HB	2.21	0.40
1:E:21:TYR:HB3	1:E:38:ASN:CG	2.46	0.40
1:A:972:THR:HG22	1:A:1035:ILE:CD1	2.51	0.40
1:C:387:TRP:CZ2	1:C:448:MET:HG2	2.56	0.40
1:C:1164:SER:O	1:C:1165:GLU:C	2.64	0.40
1:B:547:THR:HG22	1:B:561:TYR:CE1	2.57	0.40
1:D:1119:ILE:HD12	1:D:1140:ILE:HD13	2.04	0.40
1:A:1128:ASN:O	1:A:1193:THR:HB	2.21	0.40
1:B:674:THR:HG21	1:B:679:VAL:HG21	2.03	0.40
1:C:893:TYR:OH	1:C:952:ILE:HG23	2.21	0.40
1:F:113:GLY:HA3	1:F:174:ARG:HD2	2.03	0.40
1:F:591:TRP:HA	1:F:592:THR:HA	1.80	0.40
1:A:1002:TRP:CH2	1:A:1033:ALA:HB2	2.57	0.40
1:A:1123:PHE:CZ	1:A:1138:THR:HG21	2.56	0.40
1:B:881:GLY:HA3	1:B:889:ARG:HH21	1.87	0.40
1:B:1164:SER:O	1:B:1165:GLU:C	2.64	0.40
1:C:18:GLU:OE1	1:C:895:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1233/1304 (95%)	1180 (96%)	52 (4%)	1 (0%)	48	77
1	B	1229/1304 (94%)	1180 (96%)	47 (4%)	2 (0%)	43	72
1	C	1237/1304 (95%)	1186 (96%)	50 (4%)	1 (0%)	48	77
1	D	1249/1304 (96%)	1193 (96%)	53 (4%)	3 (0%)	43	72
1	E	1229/1304 (94%)	1179 (96%)	46 (4%)	4 (0%)	36	65
1	F	1238/1304 (95%)	1186 (96%)	49 (4%)	3 (0%)	43	72
All	All	7415/7824 (95%)	7104 (96%)	297 (4%)	14 (0%)	43	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1267	HIS
1	F	9	SER
1	B	663	GLY
1	D	1270	VAL
1	E	663	GLY
1	A	535	ALA
1	B	535	ALA
1	C	535	ALA
1	D	535	ALA
1	E	535	ALA
1	E	1081	ASN
1	F	535	ALA
1	E	664	SER
1	F	663	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	982/1056 (93%)	937 (95%)	45 (5%)	24	57
1	B	972/1056 (92%)	925 (95%)	47 (5%)	23	55
1	C	986/1056 (93%)	943 (96%)	43 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	989/1056 (94%)	943 (95%)	46 (5%)	23	56
1	E	960/1056 (91%)	910 (95%)	50 (5%)	21	52
1	F	983/1056 (93%)	932 (95%)	51 (5%)	21	52
All	All	5872/6336 (93%)	5590 (95%)	282 (5%)	23	55

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	33	SER
1	A	79	GLU
1	A	100	ARG
1	A	200	THR
1	A	224	ILE
1	A	227	LYS
1	A	237	THR
1	A	250	SER
1	A	260	THR
1	A	274	LYS
1	A	302	ARG
1	A	313	SER
1	A	317	GLU
1	A	471	LYS
1	A	481	TYR
1	A	499	ASN
1	A	526	SER
1	A	536	SER
1	A	543	ILE
1	A	554	SER
1	A	709	THR
1	A	748	ASN
1	A	756	THR
1	A	763	THR
1	A	772	LYS
1	A	801	ILE
1	A	818	LYS
1	A	863	LYS
1	A	870	SER
1	A	871	THR
1	A	876	THR
1	A	971	SER

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Mol	Chain	Res	Type
1	A	988	LEU
1	A	1034	THR
1	A	1035	ILE
1	A	1043	THR
1	A	1072	LYS
1	A	1078	VAL
1	A	1138	THR
1	A	1164	SER
1	A	1180	THR
1	A	1216	THR
1	A	1219	SER
1	A	1282	THR
1	B	30	ASN
1	B	33	SER
1	B	42	MET
1	B	200	THR
1	B	224	ILE
1	B	227	LYS
1	B	237	THR
1	B	260	THR
1	B	274	LYS
1	B	297	THR
1	B	302	ARG
1	B	313	SER
1	B	317	GLU
1	B	374	GLU
1	B	404	GLN
1	B	471	LYS
1	B	481	TYR
1	B	499	ASN
1	B	521	ARG
1	B	526	SER
1	B	536	SER
1	B	539	ASN
1	B	543	ILE
1	B	554	SER
1	B	662	LYS
1	B	709	THR
1	B	748	ASN
1	B	756	THR
1	B	763	THR
1	B	801	ILE

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Mol	Chain	Res	Type
1	B	863	LYS
1	B	870	SER
1	B	871	THR
1	B	876	THR
1	B	960	ASP
1	B	1040	SER
1	B	1072	LYS
1	B	1078	VAL
1	B	1138	THR
1	B	1142	ILE
1	B	1161	GLN
1	B	1164	SER
1	B	1176	PRO
1	B	1180	THR
1	B	1216	THR
1	B	1262	THR
1	B	1282	THR
1	C	33	SER
1	C	79	GLU
1	C	105	LYS
1	C	200	THR
1	C	224	ILE
1	C	227	LYS
1	C	237	THR
1	C	250	SER
1	C	260	THR
1	C	297	THR
1	C	313	SER
1	C	317	GLU
1	C	471	LYS
1	C	481	TYR
1	C	499	ASN
1	C	521	ARG
1	C	526	SER
1	C	536	SER
1	C	539	ASN
1	C	543	ILE
1	C	554	SER
1	C	709	THR
1	C	748	ASN
1	C	756	THR
1	C	763	THR

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Mol	Chain	Res	Type
1	C	767	LYS
1	C	772	LYS
1	C	801	ILE
1	C	863	LYS
1	C	870	SER
1	C	871	THR
1	C	876	THR
1	C	898	TYR
1	C	932	ASP
1	C	988	LEU
1	C	1043	THR
1	C	1072	LYS
1	C	1078	VAL
1	C	1138	THR
1	C	1164	SER
1	C	1180	THR
1	C	1216	THR
1	C	1282	THR
1	D	7	SER
1	D	8	ASP
1	D	33	SER
1	D	42	MET
1	D	47	VAL
1	D	82	SER
1	D	100	ARG
1	D	200	THR
1	D	224	ILE
1	D	237	THR
1	D	250	SER
1	D	260	THR
1	D	302	ARG
1	D	313	SER
1	D	317	GLU
1	D	471	LYS
1	D	481	TYR
1	D	521	ARG
1	D	526	SER
1	D	539	ASN
1	D	543	ILE
1	D	554	SER
1	D	620	SER
1	D	634	THR

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Mol	Chain	Res	Type
1	D	662	LYS
1	D	709	THR
1	D	748	ASN
1	D	756	THR
1	D	772	LYS
1	D	778	LYS
1	D	801	ILE
1	D	863	LYS
1	D	870	SER
1	D	871	THR
1	D	876	THR
1	D	947	VAL
1	D	971	SER
1	D	1027	LYS
1	D	1043	THR
1	D	1078	VAL
1	D	1138	THR
1	D	1164	SER
1	D	1180	THR
1	D	1216	THR
1	D	1219	SER
1	D	1282	THR
1	E	18	GLU
1	E	23	SER
1	E	30	ASN
1	E	33	SER
1	E	42	MET
1	E	100	ARG
1	E	105	LYS
1	E	200	THR
1	E	224	ILE
1	E	237	THR
1	E	250	SER
1	E	260	THR
1	E	297	THR
1	E	313	SER
1	E	317	GLU
1	E	374	GLU
1	E	404	GLN
1	E	471	LYS
1	E	481	TYR
1	E	499	ASN

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Mol	Chain	Res	Type
1	E	521	ARG
1	E	526	SER
1	E	536	SER
1	E	539	ASN
1	E	543	ILE
1	E	554	SER
1	E	662	LYS
1	E	709	THR
1	E	717	ASP
1	E	748	ASN
1	E	756	THR
1	E	763	THR
1	E	801	ILE
1	E	863	LYS
1	E	870	SER
1	E	871	THR
1	E	876	THR
1	E	946	THR
1	E	947	VAL
1	E	955	ARG
1	E	959	ILE
1	E	1034	THR
1	E	1035	ILE
1	E	1078	VAL
1	E	1138	THR
1	E	1142	ILE
1	E	1164	SER
1	E	1180	THR
1	E	1216	THR
1	E	1282	THR
1	F	7	SER
1	F	33	SER
1	F	61	GLN
1	F	79	GLU
1	F	100	ARG
1	F	105	LYS
1	F	200	THR
1	F	224	ILE
1	F	227	LYS
1	F	237	THR
1	F	250	SER
1	F	260	THR

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Mol	Chain	Res	Type
1	F	274	LYS
1	F	297	THR
1	F	313	SER
1	F	317	GLU
1	F	471	LYS
1	F	481	TYR
1	F	499	ASN
1	F	526	SER
1	F	536	SER
1	F	543	ILE
1	F	554	SER
1	F	662	LYS
1	F	709	THR
1	F	748	ASN
1	F	756	THR
1	F	763	THR
1	F	772	LYS
1	F	801	ILE
1	F	818	LYS
1	F	863	LYS
1	F	870	SER
1	F	871	THR
1	F	876	THR
1	F	947	VAL
1	F	955	ARG
1	F	957	THR
1	F	960	ASP
1	F	971	SER
1	F	988	LEU
1	F	1034	THR
1	F	1035	ILE
1	F	1072	LYS
1	F	1078	VAL
1	F	1138	THR
1	F	1164	SER
1	F	1180	THR
1	F	1216	THR
1	F	1219	SER
1	F	1282	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	499	ASN
1	A	581	GLN
1	A	639	GLN
1	A	800	HIS
1	A	896	ASN
1	B	209	ASN
1	B	499	ASN
1	B	581	GLN
1	B	639	GLN
1	B	666	ASN
1	B	711	GLN
1	B	800	HIS
1	B	896	ASN
1	B	997	ASN
1	B	1188	ASN
1	B	1217	ASN
1	B	1280	HIS
1	C	499	ASN
1	C	581	GLN
1	C	639	GLN
1	C	711	GLN
1	C	896	ASN
1	C	997	ASN
1	C	1188	ASN
1	D	581	GLN
1	D	639	GLN
1	D	711	GLN
1	D	997	ASN
1	D	1217	ASN
1	E	327	HIS
1	E	499	ASN
1	E	581	GLN
1	E	997	ASN
1	E	1188	ASN
1	E	1217	ASN
1	E	1280	HIS
1	F	499	ASN
1	F	581	GLN
1	F	639	GLN
1	F	800	HIS
1	F	1188	ASN
1	F	1217	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	2301	-	4,4,4	0.29	0	6,6,6	0.11	0
3	GOL	E	2302	-	5,5,5	0.23	0	5,5,5	0.38	0
2	SO4	F	2301	-	4,4,4	0.30	0	6,6,6	0.08	0
3	GOL	A	2303	-	5,5,5	0.20	0	5,5,5	0.63	0
2	SO4	A	2301	-	4,4,4	0.16	0	6,6,6	0.30	0
3	GOL	B	2302	-	5,5,5	0.17	0	5,5,5	0.54	0
3	GOL	C	2302	-	5,5,5	0.16	0	5,5,5	0.46	0
3	GOL	D	2302	-	5,5,5	0.14	0	5,5,5	0.48	0
3	GOL	D	2303	-	5,5,5	0.16	0	5,5,5	0.62	0
3	GOL	A	2302	-	5,5,5	0.18	0	5,5,5	0.60	0
2	SO4	D	2301	-	4,4,4	0.32	0	6,6,6	0.23	0
3	GOL	F	2302	-	5,5,5	0.08	0	5,5,5	0.44	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	GOL	E	2302	-	-	2/4/4/4	-
3	GOL	A	2303	-	-	2/4/4/4	-
3	GOL	B	2302	-	-	0/4/4/4	-
3	GOL	C	2302	-	-	2/4/4/4	-
3	GOL	D	2303	-	-	0/4/4/4	-
3	GOL	D	2302	-	-	0/4/4/4	-
3	GOL	A	2302	-	-	4/4/4/4	-
3	GOL	F	2302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2302	GOL	C1-C2-C3-O3
3	A	2303	GOL	C1-C2-C3-O3
3	A	2303	GOL	O2-C2-C3-O3
3	A	2302	GOL	O1-C1-C2-C3
3	C	2302	GOL	O1-C1-C2-C3
3	A	2302	GOL	O1-C1-C2-O2
3	A	2302	GOL	O2-C2-C3-O3
3	C	2302	GOL	O1-C1-C2-O2
3	E	2302	GOL	C1-C2-C3-O3
3	E	2302	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2302	GOL	1	0
3	B	2302	GOL	5	0
3	F	2302	GOL	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1239/1304 (95%)	-0.05	23 (1%) 66 58	55, 88, 167, 221	0
1	B	1235/1304 (94%)	-0.11	28 (2%) 61 52	48, 84, 169, 243	0
1	C	1243/1304 (95%)	-0.02	19 (1%) 72 64	59, 96, 188, 248	0
1	D	1253/1304 (96%)	0.02	22 (1%) 67 59	57, 98, 155, 227	0
1	E	1235/1304 (94%)	0.16	37 (2%) 52 43	59, 106, 248, 332	0
1	F	1244/1304 (95%)	0.36	40 (3%) 50 41	80, 148, 219, 297	0
All	All	7449/7824 (95%)	0.06	169 (2%) 61 52	48, 102, 203, 332	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	825	GLY	7.2
1	C	825	GLY	5.6
1	F	825	GLY	5.6
1	E	23	SER	4.9
1	A	11	THR	4.5
1	A	825	GLY	4.2
1	B	1262	THR	4.1
1	F	638	TYR	4.0
1	D	1268	ASP	3.9
1	E	24	ALA	3.8
1	D	539	ASN	3.8
1	D	825	GLY	3.6
1	E	634	THR	3.5
1	E	905	PRO	3.5
1	A	995	SER	3.4
1	F	1286	PHE	3.4
1	E	1108	PHE	3.4
1	B	957	THR	3.4
1	B	965	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	TRP	3.3
1	F	539	ASN	3.3
1	F	133	GLY	3.2
1	F	654	ALA	3.2
1	C	634	THR	3.2
1	A	776	ASP	3.2
1	F	537	ALA	3.2
1	D	563	ASN	3.1
1	A	1273	VAL	3.1
1	E	1186	VAL	3.1
1	E	1016	VAL	3.1
1	A	805	ALA	3.1
1	B	953	SER	3.1
1	F	575	ALA	3.1
1	A	550	GLY	3.1
1	C	1286	PHE	3.0
1	C	539	ASN	3.0
1	C	550	GLY	3.0
1	E	1195	SER	3.0
1	D	1272	ARG	3.0
1	F	357	ILE	3.0
1	E	1055	LEU	3.0
1	E	891	PHE	3.0
1	B	902	GLY	3.0
1	B	988	LEU	2.9
1	F	115	TYR	2.9
1	E	1153	ALA	2.9
1	B	1025	PHE	2.9
1	F	438	SER	2.9
1	A	1286	PHE	2.8
1	C	995	SER	2.8
1	A	292	LEU	2.8
1	C	930	VAL	2.8
1	E	996	ALA	2.8
1	D	1273	VAL	2.8
1	F	82	SER	2.8
1	F	232	PRO	2.8
1	D	807	ASN	2.7
1	B	825	GLY	2.7
1	E	998	PHE	2.7
1	E	1086	ALA	2.7
1	C	338	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1222	LEU	2.7
1	A	1003	THR	2.7
1	C	1263	VAL	2.6
1	E	1205	ILE	2.6
1	F	998	PHE	2.6
1	A	561	TYR	2.6
1	F	134	TYR	2.6
1	B	966	LEU	2.6
1	E	1071	ILE	2.6
1	D	1286	PHE	2.6
1	A	1263	VAL	2.6
1	B	550	GLY	2.6
1	F	241	ILE	2.6
1	E	965	LEU	2.5
1	C	565	ALA	2.5
1	F	135	SER	2.5
1	D	353	GLY	2.5
1	B	1286	PHE	2.5
1	F	891	PHE	2.5
1	E	1080	ALA	2.5
1	F	1159	ALA	2.5
1	B	903	ASN	2.5
1	B	1224	SER	2.5
1	B	20	VAL	2.5
1	B	987	VAL	2.4
1	F	642	TRP	2.4
1	E	950	GLN	2.4
1	E	1187	THR	2.4
1	D	536	SER	2.4
1	C	1199	CYS	2.4
1	E	1286	PHE	2.4
1	E	961	GLU	2.4
1	D	570	ALA	2.4
1	B	899	VAL	2.3
1	D	6	ARG	2.3
1	A	840	ALA	2.3
1	F	1276	GLU	2.3
1	B	581	GLN	2.3
1	A	82	SER	2.3
1	A	1110	TYR	2.3
1	D	621	TYR	2.3
1	E	1035	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	951	LYS	2.3
1	F	379	VAL	2.3
1	F	930	VAL	2.3
1	D	1267	HIS	2.3
1	D	636	TYR	2.3
1	D	801	ILE	2.3
1	A	905	PRO	2.3
1	B	539	ASN	2.3
1	E	742	GLU	2.3
1	E	332	SER	2.3
1	E	539	ASN	2.3
1	B	956	VAL	2.3
1	D	1265	PRO	2.3
1	C	963	GLY	2.3
1	B	604	ASN	2.2
1	E	1094	TRP	2.2
1	F	634	THR	2.2
1	D	7	SER	2.2
1	B	939	GLY	2.2
1	F	111	PHE	2.2
1	C	1220	ALA	2.2
1	B	1030	LYS	2.2
1	D	1269	ASN	2.2
1	A	1274	ILE	2.2
1	B	954	VAL	2.2
1	C	1273	VAL	2.2
1	A	1201	GLY	2.2
1	D	975	GLY	2.2
1	F	367	ALA	2.2
1	F	948	ALA	2.2
1	B	952	ILE	2.2
1	C	336	VAL	2.2
1	E	1121	MET	2.2
1	F	1160	ALA	2.2
1	F	114	VAL	2.2
1	F	905	PRO	2.2
1	F	1253	ALA	2.2
1	F	392	ASN	2.1
1	E	911	VAL	2.1
1	F	383	VAL	2.1
1	F	966	LEU	2.1
1	E	964	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	978	ALA	2.1
1	A	539	ASN	2.1
1	A	331	GLY	2.1
1	C	965	LEU	2.1
1	B	996	ALA	2.1
1	C	575	ALA	2.1
1	E	1106	ILE	2.1
1	E	404	GLN	2.1
1	A	930	VAL	2.1
1	E	907	LEU	2.1
1	C	811	PHE	2.1
1	F	306	PHE	2.1
1	F	14	SER	2.0
1	E	1031	VAL	2.0
1	A	807	ASN	2.0
1	E	1207	LEU	2.0
1	B	963	GLY	2.0
1	F	531	GLY	2.0
1	B	962	ILE	2.0
1	F	1017	LYS	2.0
1	D	550	GLY	2.0
1	D	1181	PHE	2.0
1	B	898	TYR	2.0
1	F	947	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	F	2301	5/5	0.71	0.09	174,178,185,188	0
3	GOL	F	2302	6/6	0.81	0.14	106,134,150,151	0
3	GOL	D	2303	6/6	0.86	0.14	92,111,124,130	0
3	GOL	C	2302	6/6	0.89	0.12	63,76,85,99	0
3	GOL	E	2302	6/6	0.89	0.20	77,100,124,196	0
3	GOL	D	2302	6/6	0.89	0.15	86,92,100,104	0
4	CA	E	2304	1/1	0.92	0.08	279,279,279,279	0
4	CA	F	2304	1/1	0.92	0.07	216,216,216,216	0
3	GOL	A	2302	6/6	0.93	0.12	48,76,85,93	0
3	GOL	B	2302	6/6	0.94	0.10	71,72,77,89	0
2	SO4	D	2301	5/5	0.94	0.08	78,107,131,132	0
3	GOL	A	2303	6/6	0.95	0.09	76,103,120,133	0
4	CA	A	2304	1/1	0.96	0.12	116,116,116,116	0
2	SO4	A	2301	5/5	0.96	0.07	54,72,83,111	0
2	SO4	C	2301	5/5	0.96	0.06	81,93,105,108	0
4	CA	C	2304	1/1	0.97	0.13	138,138,138,138	0
4	CA	B	2304	1/1	0.98	0.06	140,140,140,140	0
4	CA	D	2304	1/1	0.98	0.07	146,146,146,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.