Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:00 PM GMT

PDB ID	:	4B3K
Title	:	Family 1 6-phospho-beta-D glycosidase from Streptococcus pyogenes
Authors	:	Stepper, J.; Dabin, J.; Ekloef, J.M.; Thongpoo, P.; Kongsaeree, P.T.; Taylor, E.J.; Turkenburg, J.P.; Brumer, H.; Davies, G.J.
Deposited on	:	2012-07-24
Resolution	:	2.60 Å(reported)

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

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

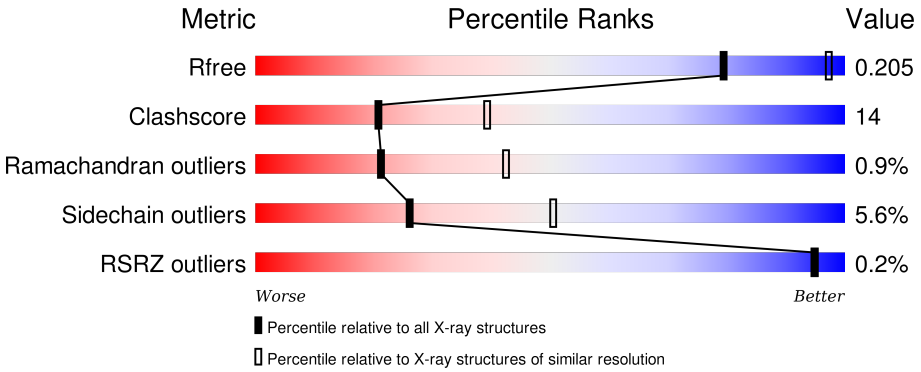
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	479	69% 24%
1	B	479	68% 26%
1	C	479	64% 29%
1	D	479	67% 25%
1	E	479	61% 32%

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Mol	Chain	Length	Quality of chain
1	F	479	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22669 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-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	B	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	C	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	D	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	E	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	F	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			

- Molecule 2 is water.

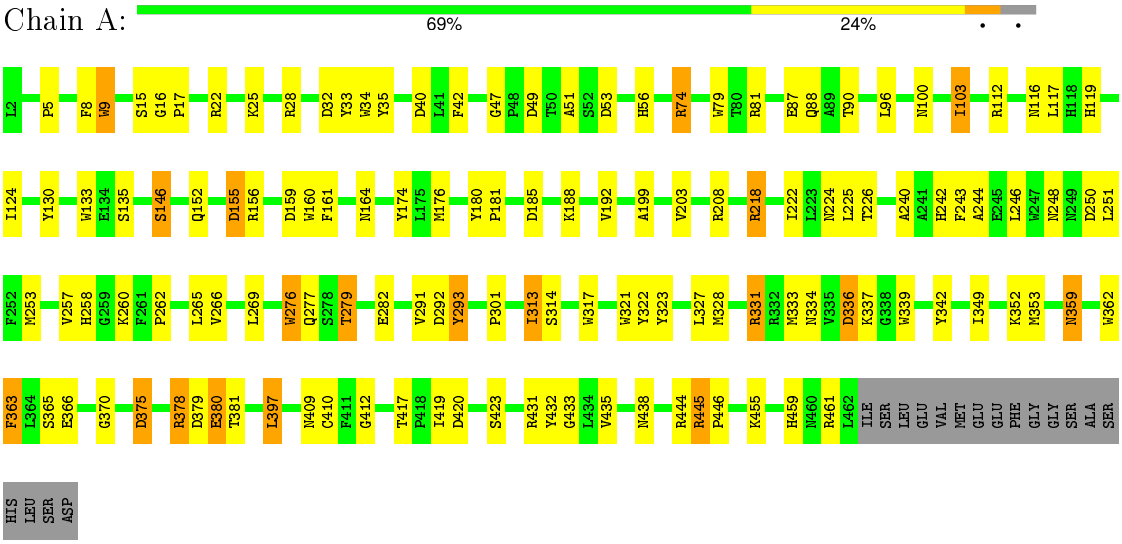
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	17	Total	O	0	0
			17	17		
2	C	10	Total	O	0	0
			10	10		
2	D	14	Total	O	0	0
			14	14		
2	E	9	Total	O	0	0
			9	9		
2	F	4	Total	O	0	0
			4	4		

3 Residue-property plots (i)

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

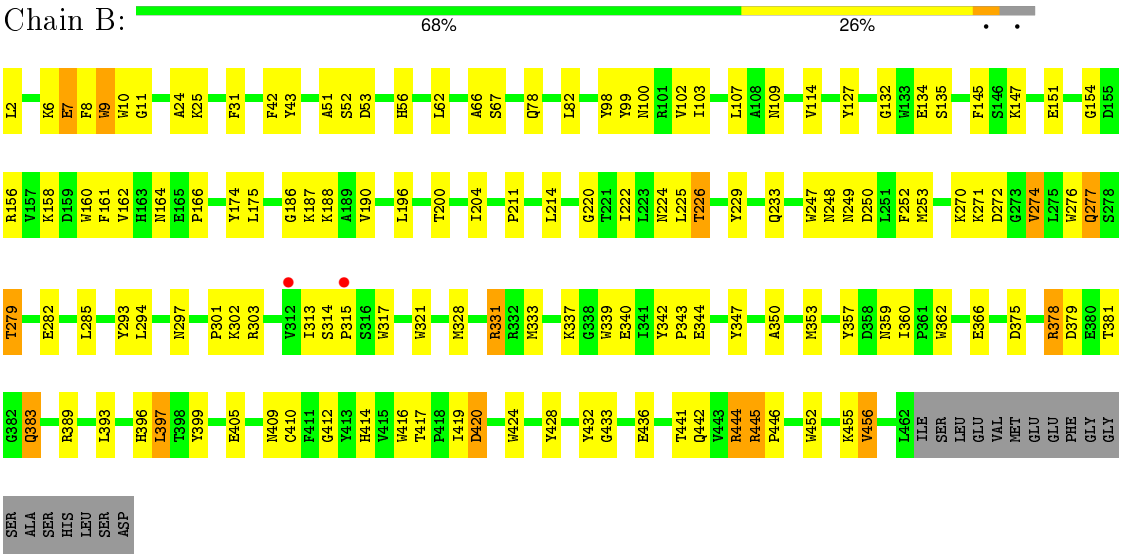
- Molecule 1: BETA-GLUCOSIDASE

Chain A:



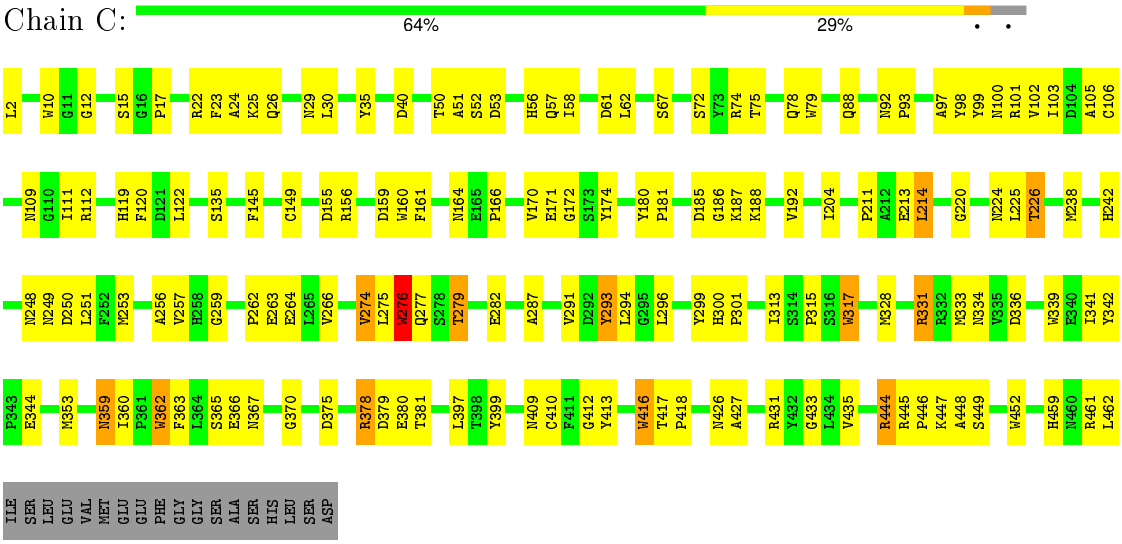
- Molecule 1: BETA-GLUCOSIDASE

Chain B:



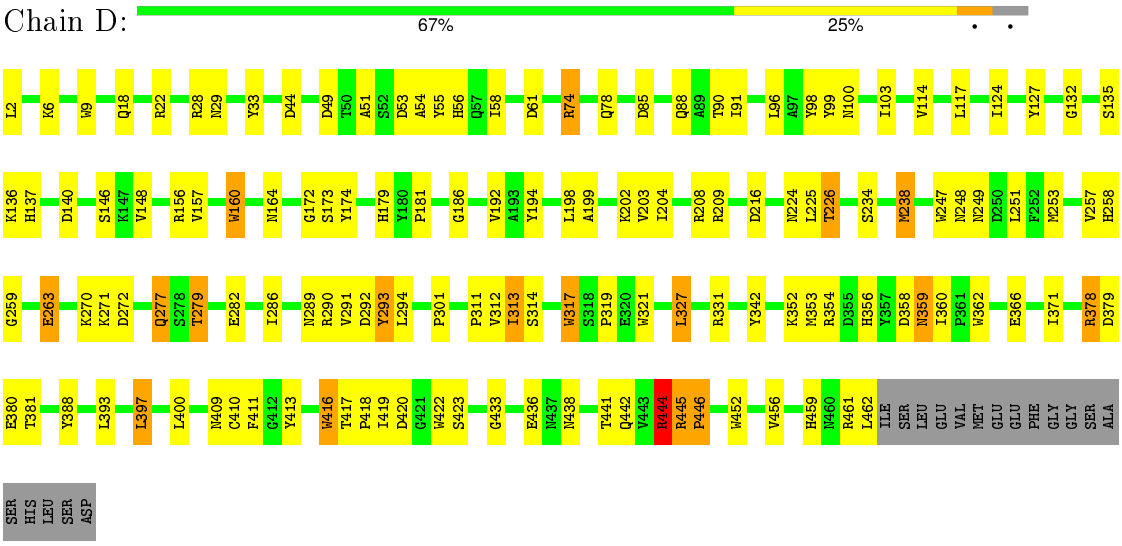
- Molecule 1: BETA-GLUCOSIDASE

Chain C:



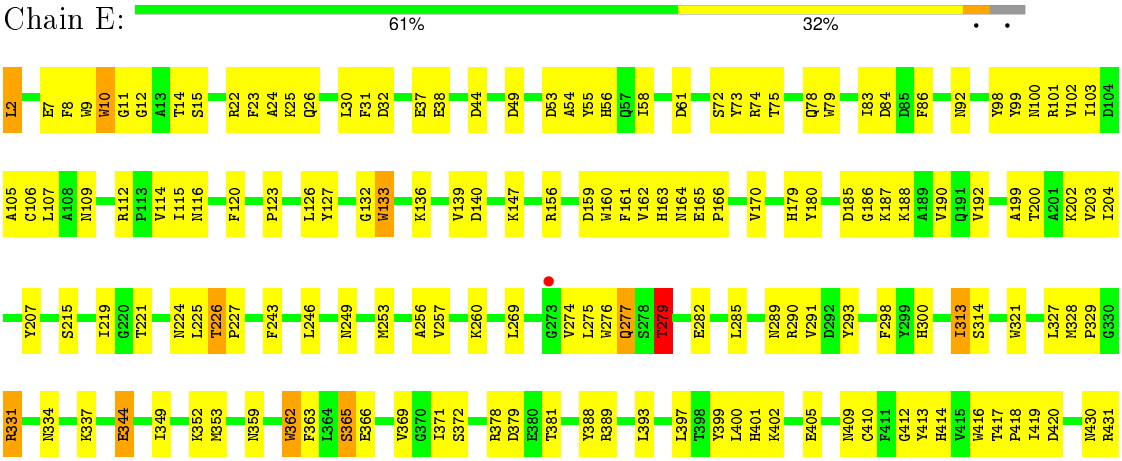
- Molecule 1: BETA-GLUCOSIDASE

Chain D:



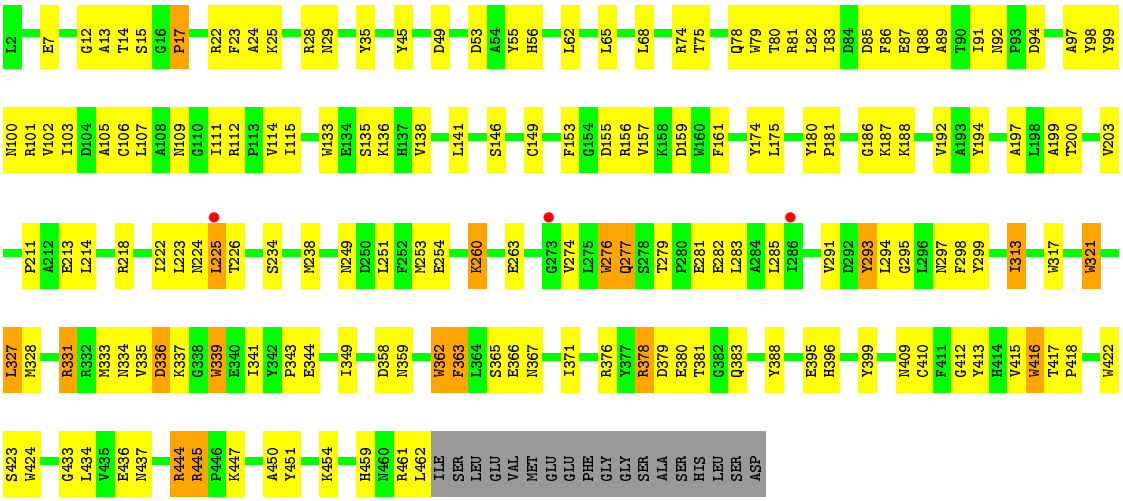
- Molecule 1: BETA-GLUCOSIDASE

Chain E:



- Molecule 1: BETA-GLUCOSIDASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.42Å 190.20Å 106.17Å 90.00° 118.88° 90.00°	Depositor
Resolution (Å)	66.56 – 2.60 66.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (66.56-2.60) 93.0 (66.56-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.223 , 0.286 0.182 , 0.205	Depositor DCC
R_{free} test set	5282 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.677 for H, K, L 0.323 for L, -K, H 0.069 for l,k,-h-l 0.069 for -h-l,k,h 0.074 for -h-l,-k,l 0.074 for h,-k,-h-l 0.348 for l,-k,h	Xtriage
Reported twinning fraction	0.677 for H, K, L 0.323 for L, -K, H	Depositor
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 105767 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22669	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.81	9/3891 (0.2%)	0.83	2/5304 (0.0%)
1	B	0.81	7/3891 (0.2%)	0.85	1/5304 (0.0%)
1	C	0.79	9/3891 (0.2%)	0.81	2/5304 (0.0%)
1	D	0.78	6/3891 (0.2%)	0.81	5/5304 (0.1%)
1	E	0.77	8/3891 (0.2%)	0.79	1/5304 (0.0%)
1	F	0.74	8/3891 (0.2%)	0.76	0/5304
All	All	0.78	47/23346 (0.2%)	0.81	11/31824 (0.0%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	133	TRP	CD2-CE2	6.40	1.49	1.41
1	D	416	TRP	CD2-CE2	6.38	1.49	1.41
1	A	34	TRP	CD2-CE2	6.27	1.48	1.41
1	B	10	TRP	CD2-CE2	6.10	1.48	1.41
1	C	79	TRP	CD2-CE2	6.07	1.48	1.41
1	D	452	TRP	CD2-CE2	6.01	1.48	1.41
1	C	339	TRP	CD2-CE2	5.99	1.48	1.41
1	A	133	TRP	CD2-CE2	5.91	1.48	1.41
1	C	362	TRP	CD2-CE2	5.88	1.48	1.41
1	F	133	TRP	CD2-CE2	5.84	1.48	1.41
1	C	160	TRP	CD2-CE2	5.82	1.48	1.41
1	F	79	TRP	CD2-CE2	5.75	1.48	1.41
1	C	416	TRP	CD2-CE2	5.75	1.48	1.41
1	D	160	TRP	CD2-CE2	5.66	1.48	1.41
1	B	9	TRP	CD2-CE2	5.61	1.48	1.41
1	C	276	TRP	CD2-CE2	5.59	1.48	1.41
1	A	317	TRP	CD2-CE2	5.55	1.48	1.41
1	F	422	TRP	CD2-CE2	5.52	1.48	1.41
1	E	79	TRP	CD2-CE2	5.50	1.48	1.41
1	B	339	TRP	CD2-CE2	5.48	1.48	1.41
1	F	416	TRP	CD2-CE2	5.47	1.48	1.41
1	A	79	TRP	CD2-CE2	5.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	362	TRP	CD2-CE2	5.39	1.47	1.41
1	D	9	TRP	CD2-CE2	5.37	1.47	1.41
1	C	452	TRP	CD2-CE2	5.35	1.47	1.41
1	A	339	TRP	CD2-CE2	5.34	1.47	1.41
1	D	317	TRP	CD2-CE2	5.33	1.47	1.41
1	F	424	TRP	CD2-CE2	5.30	1.47	1.41
1	E	276	TRP	CD2-CE2	5.28	1.47	1.41
1	B	160	TRP	CD2-CE2	5.25	1.47	1.41
1	B	247	TRP	CD2-CE2	5.24	1.47	1.41
1	A	276	TRP	CD2-CE2	5.21	1.47	1.41
1	B	452	TRP	CD2-CE2	5.20	1.47	1.41
1	E	10	TRP	CD2-CE2	5.17	1.47	1.41
1	E	452	TRP	CD2-CE2	5.17	1.47	1.41
1	F	362	TRP	CD2-CE2	5.17	1.47	1.41
1	E	321	TRP	CD2-CE2	5.16	1.47	1.41
1	F	321	TRP	CD2-CE2	5.14	1.47	1.41
1	D	321	TRP	CD2-CE2	5.13	1.47	1.41
1	F	339	TRP	CD2-CE2	5.11	1.47	1.41
1	C	317	TRP	CD2-CE2	5.08	1.47	1.41
1	A	9	TRP	CD2-CE2	5.07	1.47	1.41
1	A	160	TRP	CD2-CE2	5.04	1.47	1.41
1	C	10	TRP	CD2-CE2	5.02	1.47	1.41
1	B	276	TRP	CD2-CE2	5.01	1.47	1.41
1	A	321	TRP	CD2-CE2	5.01	1.47	1.41
1	E	160	TRP	CD2-CE2	5.00	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	444	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	250	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	444	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	28	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	C	296	LEU	CA-CB-CG	5.81	128.65	115.30
1	E	397	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	294	LEU	CA-CB-CG	5.77	128.57	115.30
1	D	354	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	327	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	40	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	96	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3767	0	3574	91	0
1	B	3767	0	3574	94	0
1	C	3767	0	3574	101	0
1	D	3767	0	3574	105	0
1	E	3767	0	3574	126	0
1	F	3767	0	3574	122	0
2	A	13	0	0	2	0
2	B	17	0	0	0	0
2	C	10	0	0	0	0
2	D	14	0	0	2	0
2	E	9	0	0	0	0
2	F	4	0	0	0	0
All	All	22669	0	21444	633	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 14.

All (633) 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:224:ASN:OD1	1:D:226:THR:HG23	1.40	1.20
1:A:224:ASN:OD1	1:A:226:THR:HG23	1.44	1.15
1:E:331:ARG:HH11	1:E:331:ARG:HG2	1.05	1.13
1:C:331:ARG:HH11	1:C:331:ARG:HG2	1.13	1.11
1:A:225:LEU:HD22	1:A:353:MET:CE	1.86	1.04
1:A:331:ARG:HH11	1:A:331:ARG:CG	1.72	1.03
1:D:225:LEU:HD22	1:D:353:MET:CE	1.91	1.01
1:A:331:ARG:HH11	1:A:331:ARG:HG3	1.22	0.99
1:A:199:ALA:O	1:A:203:VAL:HG23	1.62	0.99
1:B:224:ASN:OD1	1:B:226:THR:HG23	1.61	0.98
1:A:53:ASP:OD1	1:A:56:HIS:HD2	1.48	0.97
1:F:331:ARG:CG	1:F:331:ARG:HH11	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:ARG:CG	1:E:331:ARG:HH11	1.79	0.96
1:C:331:ARG:HH11	1:C:331:ARG:CG	1.78	0.95
1:D:225:LEU:HD22	1:D:353:MET:HE3	1.48	0.95
1:F:331:ARG:H	1:F:331:ARG:HD3	1.32	0.93
1:B:301:PRO:HG3	1:B:342:TYR:HB3	1.49	0.93
1:E:433:GLY:O	1:E:447:LYS:HD2	1.69	0.92
1:B:331:ARG:CG	1:B:331:ARG:HH11	1.80	0.92
1:C:224:ASN:OD1	1:C:226:THR:HG23	1.68	0.92
1:E:353:MET:HA	1:E:353:MET:HE2	1.49	0.91
1:B:379:ASP:OD1	1:B:381:THR:HG22	1.69	0.91
1:F:224:ASN:OD1	1:F:226:THR:HG23	1.70	0.91
1:E:359:ASN:HD21	1:E:409:ASN:H	1.17	0.91
1:F:114:VAL:O	1:F:115:ILE:HD13	1.69	0.90
1:D:379:ASP:OD1	1:D:381:THR:HG22	1.72	0.89
1:D:301:PRO:HG3	1:D:342:TYR:HB3	1.51	0.89
1:E:56:HIS:CD2	1:F:56:HIS:CD2	2.62	0.87
1:F:331:ARG:HH11	1:F:331:ARG:HG3	1.40	0.86
1:E:105:ALA:O	1:E:109:ASN:ND2	2.08	0.86
1:D:291:VAL:HG21	1:D:294:LEU:HD21	1.58	0.86
1:B:331:ARG:HG2	1:B:331:ARG:HH11	1.41	0.84
1:E:99:TYR:O	1:E:103:ILE:HG12	1.76	0.84
1:E:381:THR:O	1:E:445:ARG:NH2	2.12	0.83
1:C:328:MET:O	1:C:331:ARG:HD2	1.78	0.83
1:A:53:ASP:OD1	1:A:56:HIS:CD2	2.33	0.82
1:F:328:MET:O	1:F:331:ARG:HD2	1.79	0.82
1:C:53:ASP:OD1	1:C:56:HIS:HD2	1.63	0.81
1:F:199:ALA:O	1:F:203:VAL:HG23	1.81	0.81
1:D:418:PRO:HD2	2:D:2012:HOH:O	1.81	0.81
1:A:225:LEU:HD22	1:A:353:MET:HE2	1.63	0.81
1:B:359:ASN:HD21	1:B:409:ASN:H	1.28	0.81
1:F:22:ARG:NH2	1:F:28:ARG:HG2	1.98	0.79
1:E:328:MET:O	1:E:331:ARG:HD2	1.83	0.79
1:D:291:VAL:HG21	1:D:294:LEU:CD2	2.13	0.78
1:E:331:ARG:NH1	1:E:331:ARG:HG2	1.86	0.78
1:C:100:ASN:HD22	1:C:156:ARG:HH12	1.30	0.78
1:F:105:ALA:O	1:F:109:ASN:ND2	2.15	0.78
1:E:56:HIS:HD2	1:F:56:HIS:NE2	1.82	0.77
1:A:225:LEU:CD2	1:A:353:MET:HE2	2.15	0.77
1:E:256:ALA:O	1:E:291:VAL:HG22	1.84	0.77
1:A:328:MET:O	1:A:331:ARG:HD3	1.86	0.76
1:D:379:ASP:CG	1:D:381:THR:HG22	2.05	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:NH1	1:C:331:ARG:HG2	1.94	0.76
1:F:159:ASP:OD1	1:F:218:ARG:HD3	1.87	0.75
1:F:328:MET:O	1:F:331:ARG:CD	2.35	0.75
1:C:299:TYR:OH	1:C:366:GLU:OE1	2.04	0.74
1:C:225:LEU:HD22	1:C:353:MET:HE3	1.70	0.74
1:C:225:LEU:HD13	1:C:253:MET:HG3	1.70	0.74
1:D:225:LEU:HD22	1:D:353:MET:HE2	1.70	0.74
1:A:359:ASN:HD21	1:A:409:ASN:H	1.35	0.73
1:B:6:LYS:O	1:B:7:GLU:HB2	1.85	0.73
1:C:328:MET:O	1:C:331:ARG:CD	2.35	0.73
1:F:223:LEU:HD12	1:F:253:MET:SD	2.28	0.73
1:C:291:VAL:HB	1:C:293:TYR:O	1.89	0.73
1:A:225:LEU:HD13	1:A:253:MET:HG3	1.70	0.73
1:F:379:ASP:OD1	1:F:381:THR:HG22	1.89	0.73
1:F:281:GLU:O	1:F:285:LEU:HG	1.89	0.72
1:B:248:ASN:C	1:B:249:ASN:HD22	1.92	0.72
1:A:375:ASP:O	1:A:378:ARG:HG2	1.88	0.72
1:C:25:LYS:HZ1	1:C:78:GLN:HE22	1.36	0.72
1:E:22:ARG:HD3	1:E:49:ASP:OD1	1.90	0.72
1:F:331:ARG:CG	1:F:331:ARG:NH1	2.48	0.71
1:E:140:ASP:OD1	1:E:202:LYS:NZ	2.21	0.71
1:D:127:TYR:CZ	1:D:181:PRO:HG3	2.25	0.71
1:E:56:HIS:HD2	1:F:56:HIS:CD2	2.08	0.71
1:E:224:ASN:OD1	1:E:226:THR:HG23	1.90	0.71
1:D:225:LEU:CD2	1:D:353:MET:CE	2.68	0.70
1:A:301:PRO:HG3	1:A:342:TYR:HB3	1.73	0.70
1:A:103:ILE:N	1:A:103:ILE:HD13	2.06	0.70
1:A:279:THR:HG22	1:A:282:GLU:H	1.56	0.70
1:F:331:ARG:HD3	1:F:331:ARG:N	2.04	0.70
1:A:331:ARG:CG	1:A:331:ARG:NH1	2.40	0.70
1:F:359:ASN:HD21	1:F:409:ASN:H	1.39	0.70
1:E:26:GLN:OE1	1:E:92:ASN:ND2	2.24	0.69
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.58	0.69
1:C:459:HIS:O	1:C:461:ARG:HG3	1.93	0.69
1:D:253:MET:HE1	1:D:353:MET:HE1	1.75	0.68
1:D:225:LEU:CD2	1:D:353:MET:HE3	2.22	0.68
1:F:13:ALA:HB1	1:F:74:ARG:NH1	2.09	0.67
1:C:25:LYS:NZ	1:C:78:GLN:HE22	1.90	0.67
1:E:204:ILE:HA	1:E:219:ILE:HD13	1.77	0.67
1:A:225:LEU:HD21	1:A:352:LYS:HG2	1.77	0.67
1:D:253:MET:CE	1:D:353:MET:CE	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:TYR:O	1:F:103:ILE:HG12	1.95	0.67
1:F:78:GLN:HB2	1:F:99:TYR:OH	1.93	0.67
1:B:389:ARG:O	1:B:393:LEU:HG	1.95	0.67
1:B:53:ASP:OD1	1:B:56:HIS:HD2	1.78	0.66
1:D:253:MET:CE	1:D:353:MET:HE1	2.24	0.66
1:A:225:LEU:HD22	1:A:353:MET:HE3	1.74	0.66
1:E:279:THR:HG22	1:E:282:GLU:H	1.60	0.66
1:C:30:LEU:HD21	1:C:122:LEU:HD23	1.77	0.66
1:E:269:LEU:HB2	1:E:275:LEU:CD1	2.25	0.66
1:E:207:TYR:O	1:E:215:SER:HB3	1.95	0.66
1:D:99:TYR:O	1:D:103:ILE:HG12	1.95	0.66
1:E:257:VAL:O	1:E:290:ARG:HD3	1.95	0.65
1:C:225:LEU:HD22	1:C:353:MET:CE	2.26	0.65
1:E:98:TYR:O	1:E:102:VAL:HG23	1.97	0.65
1:A:100:ASN:HD22	1:A:156:ARG:HH12	1.42	0.65
1:B:441:THR:O	1:B:442:GLN:HB2	1.95	0.65
1:B:417:THR:O	1:B:433:GLY:HA2	1.97	0.65
1:A:225:LEU:O	1:A:349:ILE:HG12	1.97	0.64
1:D:253:MET:HE2	1:D:353:MET:HE2	1.78	0.64
1:E:353:MET:CE	1:E:353:MET:HA	2.23	0.64
1:D:127:TYR:CE1	1:D:181:PRO:HG3	2.32	0.64
1:E:199:ALA:O	1:E:203:VAL:HG23	1.97	0.64
1:F:381:THR:O	1:F:445:ARG:NH2	2.30	0.64
1:D:136:LYS:NZ	1:D:282:GLU:OE1	2.31	0.64
1:A:188:LYS:O	1:A:192:VAL:HG23	1.98	0.64
1:F:379:ASP:CG	1:F:381:THR:HG22	2.17	0.64
1:A:301:PRO:HG3	1:A:342:TYR:CB	2.28	0.64
1:E:186:GLY:O	1:E:190:VAL:HG23	1.98	0.64
1:E:188:LYS:O	1:E:192:VAL:HG23	1.97	0.64
1:B:416:TRP:CD1	1:B:417:THR:HB	2.33	0.63
1:A:417:THR:O	1:A:433:GLY:HA2	1.97	0.63
1:D:53:ASP:OD1	1:D:56:HIS:HD2	1.82	0.63
1:A:337:LYS:HE3	1:A:432:TYR:OH	1.98	0.63
1:A:225:LEU:CD2	1:A:353:MET:CE	2.66	0.63
1:B:331:ARG:NH1	1:B:331:ARG:HG2	2.03	0.63
1:C:100:ASN:ND2	1:C:156:ARG:HH12	1.97	0.63
1:F:331:ARG:HG2	1:F:331:ARG:HH11	1.62	0.63
1:D:359:ASN:HD21	1:D:409:ASN:H	1.48	0.62
1:C:256:ALA:O	1:C:291:VAL:HG22	2.00	0.62
1:A:100:ASN:HD21	1:A:156:ARG:HH22	1.48	0.62
1:D:279:THR:HG22	1:D:282:GLU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASP:OD2	1:D:88:GLN:HG2	1.99	0.61
1:A:15:SER:HB3	1:A:119:HIS:CD2	2.35	0.61
1:E:9:TRP:HB2	1:E:412:GLY:HA3	1.82	0.61
1:A:331:ARG:HH11	1:A:331:ARG:HG2	1.65	0.61
1:E:185:ASP:HB3	1:E:188:LYS:HD2	1.81	0.61
1:E:26:GLN:HE22	1:E:84:ASP:HA	1.66	0.61
1:F:279:THR:HB	1:F:282:GLU:HG3	1.83	0.61
1:A:328:MET:O	1:A:331:ARG:CD	2.48	0.61
1:F:149:CYS:O	1:F:153:PHE:HD2	1.83	0.61
1:D:225:LEU:CD2	1:D:353:MET:HE2	2.31	0.61
1:B:279:THR:HG22	1:B:282:GLU:H	1.64	0.61
1:E:393:LEU:HD22	1:E:413:TYR:OH	1.99	0.61
1:E:100:ASN:ND2	1:E:156:ARG:HH22	1.99	0.61
1:C:26:GLN:OE1	1:C:92:ASN:ND2	2.30	0.61
1:C:331:ARG:NH1	1:C:331:ARG:CG	2.45	0.61
1:E:221:THR:HG22	1:E:291:VAL:HG11	1.82	0.61
1:E:433:GLY:O	1:E:447:LYS:CD	2.47	0.60
1:F:25:LYS:HE3	1:F:80:THR:OG1	2.01	0.60
1:F:103:ILE:HD12	1:F:157:VAL:CG2	2.32	0.60
1:C:359:ASN:HD21	1:C:409:ASN:H	1.47	0.60
1:A:25:LYS:HG3	1:A:81:ARG:HB2	1.82	0.60
1:B:225:LEU:CD2	1:B:353:MET:HE2	2.31	0.60
1:D:253:MET:HE1	1:D:353:MET:CE	2.32	0.60
1:D:293:TYR:O	1:D:294:LEU:HD23	2.02	0.60
1:B:331:ARG:NH1	1:B:331:ARG:CG	2.49	0.60
1:D:378:ARG:HH22	1:D:436:GLU:CD	2.05	0.59
1:E:225:LEU:HD21	1:E:352:LYS:HG2	1.84	0.59
1:E:107:LEU:HD11	1:E:156:ARG:HB3	1.82	0.59
1:F:107:LEU:HD11	1:F:156:ARG:HB3	1.84	0.59
1:A:224:ASN:OD1	1:A:226:THR:CG2	2.35	0.59
1:C:100:ASN:ND2	1:C:156:ARG:HH22	2.00	0.59
1:F:112:ARG:HD3	1:F:159:ASP:OD2	2.03	0.59
1:F:149:CYS:O	1:F:153:PHE:CD2	2.55	0.59
1:E:331:ARG:CG	1:E:331:ARG:NH1	2.44	0.59
1:C:242:HIS:HE2	1:C:264:GLU:CD	2.06	0.59
1:E:451:TYR:O	1:E:454:LYS:HB3	2.03	0.59
1:E:353:MET:CA	1:E:353:MET:HE2	2.28	0.59
1:B:98:TYR:O	1:B:102:VAL:HG23	2.03	0.59
1:F:291:VAL:HB	1:F:293:TYR:O	2.03	0.59
1:A:116:ASN:HA	1:A:161:PHE:O	2.03	0.58
1:E:8:PHE:HD2	1:E:10:TRP:CZ2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:THR:HG22	1:C:282:GLU:H	1.68	0.58
1:E:225:LEU:HD21	1:E:352:LYS:HB3	1.85	0.58
1:F:254:GLU:HB3	1:F:260:LYS:O	2.03	0.58
1:D:22:ARG:NH2	1:D:28:ARG:HG2	2.18	0.58
1:D:253:MET:HE2	1:D:353:MET:CE	2.33	0.58
1:E:269:LEU:HB2	1:E:275:LEU:HD13	1.85	0.58
1:E:185:ASP:CB	1:E:188:LYS:HD2	2.34	0.58
1:B:328:MET:O	1:B:331:ARG:HD3	2.04	0.58
1:D:411:PHE:O	1:D:411:PHE:HD1	1.87	0.58
1:B:154:GLY:O	1:B:158:LYS:NZ	2.33	0.58
1:C:105:ALA:O	1:C:109:ASN:ND2	2.35	0.58
1:C:435:VAL:HA	1:C:446:PRO:HA	1.86	0.58
1:F:378:ARG:NH2	1:F:436:GLU:OE1	2.37	0.57
1:C:100:ASN:HD22	1:C:156:ARG:NH1	1.99	0.57
1:F:180:TYR:CG	1:F:181:PRO:HA	2.38	0.57
1:E:371:ILE:HG13	1:E:388:TYR:CE1	2.38	0.57
1:A:174:TYR:CE2	1:A:192:VAL:HG21	2.39	0.57
1:A:88:GLN:HB2	1:A:90:THR:HG23	1.86	0.57
1:A:331:ARG:NH1	1:A:331:ARG:HG3	2.02	0.57
1:F:371:ILE:HG13	1:F:388:TYR:CE1	2.40	0.57
1:D:301:PRO:CG	1:D:342:TYR:HB3	2.30	0.57
1:F:13:ALA:CB	1:F:74:ARG:NH1	2.68	0.57
1:A:359:ASN:ND2	1:A:409:ASN:H	2.02	0.57
1:A:103:ILE:HD13	1:A:103:ILE:H	1.69	0.56
1:E:344:GLU:HG3	1:E:399:TYR:CZ	2.41	0.56
1:D:417:THR:O	1:D:433:GLY:HA2	2.05	0.56
1:E:400:LEU:HD11	1:E:410:CYS:SG	2.45	0.56
1:B:25:LYS:NZ	1:B:78:GLN:HE22	2.03	0.56
1:F:378:ARG:HA	1:F:383:GLN:O	2.06	0.56
1:F:155:ASP:OD2	1:F:156:ARG:NE	2.35	0.56
1:A:96:LEU:HD11	1:A:152:GLN:HE21	1.69	0.56
1:D:257:VAL:HG22	1:D:360:ILE:HD13	1.87	0.56
1:B:301:PRO:HG3	1:B:342:TYR:CB	2.30	0.56
1:A:155:ASP:HB3	1:D:459:HIS:CE1	2.41	0.56
1:F:417:THR:O	1:F:433:GLY:HA2	2.06	0.56
1:E:362:TRP:O	1:E:410:CYS:HA	2.06	0.56
1:B:82:LEU:HD23	1:B:145:PHE:HE1	1.71	0.56
1:C:98:TYR:O	1:C:101:ARG:HB2	2.05	0.56
1:B:375:ASP:O	1:B:378:ARG:HG2	2.06	0.56
1:B:297:ASN:ND2	1:B:366:GLU:HB2	2.21	0.55
1:C:97:ALA:O	1:C:101:ARG:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:GLU:HG2	1:E:416:TRP:HE3	1.72	0.55
1:C:334:ASN:HB2	1:C:341:ILE:HD11	1.88	0.55
1:D:411:PHE:CD1	1:D:411:PHE:O	2.59	0.55
1:A:199:ALA:O	1:A:203:VAL:CG2	2.47	0.55
1:C:362:TRP:CE2	1:C:410:CYS:HB2	2.42	0.55
1:C:100:ASN:HD21	1:C:156:ARG:HH22	1.54	0.55
1:B:162:VAL:HG11	1:B:200:THR:HA	1.88	0.55
1:A:331:ARG:NH1	1:A:331:ARG:HG2	2.19	0.55
1:D:257:VAL:O	1:D:290:ARG:HD3	2.07	0.55
1:C:98:TYR:HA	1:C:101:ARG:HD3	1.88	0.55
1:A:363:PHE:CZ	1:A:365:SER:HB3	2.42	0.55
1:F:234:SER:O	1:F:238:MET:HB2	2.06	0.55
1:D:251:LEU:HD23	1:D:251:LEU:C	2.27	0.55
1:C:362:TRP:O	1:C:410:CYS:HA	2.05	0.55
1:F:222:ILE:HG12	1:F:295:GLY:HA3	1.89	0.55
1:D:253:MET:CE	1:D:353:MET:HE2	2.36	0.54
1:E:100:ASN:HD21	1:E:156:ARG:HH22	1.55	0.54
1:F:363:PHE:HB2	1:F:412:GLY:O	2.07	0.54
1:A:459:HIS:HB3	1:A:461:ARG:HE	1.72	0.54
1:E:359:ASN:ND2	1:E:409:ASN:H	1.95	0.54
1:A:100:ASN:ND2	1:A:156:ARG:HH12	2.05	0.54
1:F:82:LEU:O	1:F:92:ASN:HB3	2.07	0.54
1:E:225:LEU:O	1:E:225:LEU:HG	2.07	0.54
1:B:6:LYS:O	1:B:7:GLU:CB	2.53	0.54
1:E:114:VAL:O	1:E:115:ILE:HD13	2.08	0.54
1:B:211:PRO:HG2	1:B:214:LEU:HD12	1.89	0.54
1:F:98:TYR:O	1:F:102:VAL:HG23	2.07	0.54
1:A:22:ARG:N	1:A:49:ASP:O	2.28	0.54
1:F:12:GLY:HA3	1:F:418:PRO:HG3	1.89	0.54
1:E:112:ARG:HD3	1:E:159:ASP:OD2	2.08	0.54
1:F:114:VAL:CG1	1:F:161:PHE:HE2	2.20	0.54
1:D:172:GLY:C	1:D:179:HIS:HB2	2.29	0.54
1:D:74:ARG:HB2	1:D:114:VAL:HB	1.89	0.54
1:A:379:ASP:OD1	1:A:381:THR:HG22	2.07	0.54
1:A:362:TRP:O	1:A:410:CYS:HA	2.08	0.53
1:B:100:ASN:HD22	1:B:156:ARG:HH12	1.56	0.53
1:E:8:PHE:CD2	1:E:10:TRP:CZ2	2.95	0.53
1:A:9:TRP:HB2	1:A:412:GLY:HA3	1.90	0.53
1:E:225:LEU:HD22	1:E:353:MET:HE3	1.91	0.53
1:F:451:TYR:O	1:F:454:LYS:HB3	2.08	0.53
1:B:174:TYR:O	1:B:175:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:TRP:CZ2	1:E:410:CYS:HB2	2.44	0.53
1:F:94:ASP:O	1:F:97:ALA:HB3	2.09	0.53
1:A:250:ASP:O	1:A:251:LEU:C	2.45	0.53
1:A:35:TYR:CD2	1:A:47:GLY:HA3	2.43	0.53
1:B:134:GLU:OE1	1:B:188:LYS:HE2	2.09	0.53
1:B:379:ASP:CG	1:B:381:THR:HG22	2.28	0.53
1:D:379:ASP:OD2	1:D:381:THR:HG22	2.08	0.53
1:D:88:GLN:HB2	1:D:90:THR:HG23	1.90	0.53
1:C:23:PHE:O	1:C:25:LYS:N	2.42	0.52
1:D:74:ARG:NH2	1:D:164:ASN:OD1	2.40	0.52
1:A:240:ALA:HB1	1:A:323:TYR:HB3	1.90	0.52
1:E:136:LYS:NZ	1:E:277:GLN:O	2.41	0.52
1:E:11:GLY:O	1:E:414:HIS:HA	2.09	0.52
1:B:166:PRO:HB2	1:B:252:PHE:CZ	2.44	0.52
1:E:98:TYR:O	1:E:101:ARG:HB2	2.10	0.52
1:F:100:ASN:HD21	1:F:156:ARG:HH22	1.58	0.52
1:A:33:TYR:CG	1:A:124:ILE:HG12	2.44	0.52
1:F:81:ARG:HG3	1:F:81:ARG:HH11	1.73	0.52
1:F:53:ASP:OD1	1:F:56:HIS:HD2	1.93	0.52
1:C:112:ARG:HD3	1:C:159:ASP:OD2	2.09	0.52
1:C:262:PRO:O	1:C:266:VAL:HG23	2.10	0.52
1:C:248:ASN:C	1:C:249:ASN:HD22	2.13	0.52
1:F:335:VAL:O	1:F:337:LYS:N	2.43	0.52
1:D:259:GLY:O	1:D:286:ILE:HG22	2.09	0.52
1:F:459:HIS:O	1:F:461:ARG:HG3	2.10	0.52
1:A:117:LEU:HD13	1:A:146:SER:HB3	1.92	0.52
1:E:300:HIS:O	1:E:300:HIS:ND1	2.43	0.52
1:C:99:TYR:O	1:C:102:VAL:HB	2.10	0.52
1:C:362:TRP:CZ2	1:C:410:CYS:HB2	2.45	0.51
1:F:97:ALA:O	1:F:101:ARG:HG3	2.10	0.51
1:C:22:ARG:O	1:D:441:THR:HA	2.09	0.51
1:C:379:ASP:OD1	1:C:381:THR:HG22	2.10	0.51
1:E:226:THR:HA	1:E:349:ILE:HD11	1.93	0.51
1:F:416:TRP:CD1	1:F:417:THR:HB	2.45	0.51
1:F:297:ASN:ND2	1:F:366:GLU:HG3	2.24	0.51
1:F:434:LEU:HB3	1:F:450:ALA:HB2	1.93	0.51
1:E:378:ARG:NH2	1:E:436:GLU:OE2	2.40	0.51
1:F:225:LEU:HB3	1:F:349:ILE:HG12	1.93	0.51
1:B:381:THR:HG23	1:B:383:GLN:HB2	1.93	0.51
1:C:187:LYS:HA	1:C:274:VAL:HG22	1.92	0.51
1:E:416:TRP:CD1	1:E:417:THR:HB	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:TYR:CE2	1:D:192:VAL:HG21	2.46	0.51
1:F:331:ARG:HG2	1:F:331:ARG:NH1	2.23	0.51
1:E:53:ASP:C	1:E:55:TYR:H	2.14	0.51
1:D:136:LYS:HZ3	1:D:282:GLU:CD	2.14	0.51
1:B:11:GLY:O	1:B:414:HIS:HA	2.11	0.51
1:B:337:LYS:HE3	1:B:432:TYR:OH	2.10	0.51
1:F:29:ASN:ND2	1:F:78:GLN:HE21	2.09	0.51
1:C:185:ASP:CG	1:C:188:LYS:HG3	2.31	0.50
1:C:88:GLN:OE1	1:C:88:GLN:HA	2.11	0.50
1:F:194:TYR:HB2	1:F:276:TRP:CE3	2.46	0.50
1:F:211:PRO:HD2	1:F:214:LEU:HD12	1.93	0.50
1:A:242:HIS:CE1	2:A:2008:HOH:O	2.64	0.50
1:C:213:GLU:HG2	1:C:214:LEU:HG	1.93	0.50
1:E:2:LEU:HG	1:E:401:HIS:ND1	2.26	0.50
1:C:367:ASN:ND2	1:C:413:TYR:OH	2.38	0.50
1:E:162:VAL:HG11	1:E:200:THR:HA	1.92	0.50
1:E:25:LYS:HZ2	1:E:78:GLN:HE22	1.58	0.50
1:C:106:CYS:HB3	1:C:111:ILE:O	2.11	0.50
1:C:99:TYR:O	1:C:103:ILE:HG12	2.11	0.50
1:B:381:THR:O	1:B:445:ARG:NH2	2.43	0.50
1:F:25:LYS:HB2	1:F:81:ARG:HH12	1.76	0.50
1:A:246:LEU:HA	1:A:250:ASP:HB2	1.94	0.50
1:C:211:PRO:HG2	1:C:214:LEU:HD12	1.93	0.50
1:B:366:GLU:HG2	1:B:416:TRP:HE3	1.76	0.50
1:C:53:ASP:OD1	1:C:56:HIS:CD2	2.54	0.50
1:C:72:SER:HA	1:C:112:ARG:O	2.11	0.50
1:E:61:ASP:OD1	1:E:444:ARG:HD2	2.12	0.50
1:D:74:ARG:HA	1:D:114:VAL:O	2.12	0.50
1:A:380:GLU:HG2	1:A:381:THR:N	2.26	0.50
1:D:199:ALA:O	1:D:203:VAL:HG23	2.12	0.50
1:D:29:ASN:HD22	1:D:78:GLN:NE2	2.10	0.49
1:E:243:PHE:HA	1:E:246:LEU:HD12	1.94	0.49
1:B:419:ILE:O	1:B:420:ASP:C	2.49	0.49
1:C:61:ASP:OD1	1:C:444:ARG:HD2	2.12	0.49
1:A:100:ASN:ND2	1:A:156:ARG:HH22	2.10	0.49
1:D:393:LEU:O	1:D:397:LEU:HB2	2.12	0.49
1:D:117:LEU:HD13	1:D:146:SER:HB2	1.93	0.49
1:F:251:LEU:C	1:F:251:LEU:HD23	2.33	0.49
1:F:249:ASN:O	1:F:253:MET:HB2	2.12	0.49
1:B:82:LEU:HD23	1:B:145:PHE:CE1	2.48	0.49
1:E:402:LYS:O	1:E:405:GLU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:N	1:B:103:ILE:HD13	2.26	0.49
1:D:371:ILE:HG13	1:D:388:TYR:CE2	2.47	0.49
1:E:73:TYR:CE2	1:E:75:THR:HB	2.48	0.49
1:F:433:GLY:O	1:F:447:LYS:HD2	2.13	0.49
1:B:147:LYS:NZ	1:B:151:GLU:OE2	2.45	0.49
1:D:2:LEU:HD23	1:D:462:LEU:HD12	1.94	0.49
1:A:265:LEU:O	1:A:269:LEU:HG	2.12	0.49
1:D:157:VAL:HB	1:D:160:TRP:CZ2	2.47	0.49
1:C:166:PRO:O	1:C:170:VAL:HG23	2.13	0.49
1:B:294:LEU:O	1:B:362:TRP:HA	2.13	0.49
1:C:15:SER:HB2	1:C:17:PRO:HD2	1.95	0.49
1:C:328:MET:O	1:C:331:ARG:HD3	2.12	0.48
1:B:253:MET:CE	1:B:353:MET:CE	2.91	0.48
1:E:136:LYS:O	1:E:139:VAL:HB	2.13	0.48
1:B:31:PHE:CE2	1:B:424:TRP:CE3	3.00	0.48
1:C:359:ASN:ND2	1:C:409:ASN:H	2.11	0.48
1:E:372:SER:HB3	1:E:430:ASN:HD22	1.77	0.48
1:C:331:ARG:HH12	1:C:333:MET:HB2	1.79	0.48
1:E:417:THR:O	1:E:433:GLY:HA2	2.13	0.48
1:E:55:TYR:HD2	1:E:56:HIS:ND1	2.12	0.48
1:E:74:ARG:HH12	1:E:366:GLU:HG3	1.79	0.48
1:E:74:ARG:NH1	1:E:366:GLU:HG3	2.28	0.48
1:A:379:ASP:O	1:A:380:GLU:C	2.52	0.48
1:F:367:ASN:ND2	1:F:413:TYR:OH	2.44	0.48
1:F:344:GLU:HG3	1:F:399:TYR:CZ	2.48	0.48
1:C:29:ASN:HD22	1:C:78:GLN:NE2	2.12	0.48
1:A:363:PHE:HB2	1:A:412:GLY:O	2.14	0.48
1:F:331:ARG:HG3	1:F:331:ARG:NH1	2.20	0.47
1:D:362:TRP:O	1:D:410:CYS:HA	2.15	0.47
1:A:112:ARG:HD3	1:A:159:ASP:OD2	2.14	0.47
1:F:328:MET:O	1:F:331:ARG:HD3	2.13	0.47
1:C:29:ASN:HD22	1:C:78:GLN:HE21	1.60	0.47
1:F:136:LYS:NZ	1:F:282:GLU:OE1	2.46	0.47
1:E:300:HIS:O	1:E:300:HIS:CG	2.68	0.47
1:C:301:PRO:HG3	1:C:342:TYR:HB3	1.95	0.47
1:D:61:ASP:OD1	1:D:444:ARG:HD2	2.13	0.47
1:A:333:MET:HG3	1:A:334:ASN:N	2.29	0.47
1:B:331:ARG:NH2	1:B:333:MET:SD	2.77	0.47
1:D:379:ASP:OD1	1:D:381:THR:CG2	2.54	0.47
1:F:379:ASP:OD1	1:F:381:THR:CG2	2.60	0.47
1:E:54:ALA:O	1:E:58:ILE:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:HG3	1:B:399:TYR:CE1	2.50	0.47
1:D:352:LYS:HE3	1:D:356:HIS:HB2	1.96	0.47
1:E:313:ILE:HD13	1:E:314:SER:N	2.30	0.47
1:D:204:ILE:CG2	1:D:289:ASN:HB3	2.44	0.47
1:D:204:ILE:HG22	1:D:289:ASN:HB3	1.95	0.47
1:E:269:LEU:HB2	1:E:275:LEU:HD12	1.96	0.47
1:B:343:PRO:HB3	1:B:396:HIS:CE1	2.49	0.47
1:F:106:CYS:HB3	1:F:111:ILE:O	2.14	0.47
1:F:135:SER:HB3	1:F:138:VAL:HG23	1.97	0.47
1:C:426:ASN:O	1:C:427:ALA:C	2.53	0.47
1:F:313:ILE:HD13	1:F:313:ILE:HA	1.67	0.47
1:A:370:GLY:HA2	1:A:431:ARG:O	2.15	0.47
1:F:327:LEU:N	1:F:327:LEU:HD22	2.29	0.47
1:F:317:TRP:HA	1:F:321:TRP:CZ2	2.50	0.47
1:C:448:ALA:O	1:C:449:SER:C	2.51	0.47
1:B:445:ARG:O	1:B:446:PRO:C	2.54	0.46
1:C:2:LEU:HD23	1:C:462:LEU:HD12	1.97	0.46
1:C:174:TYR:CE2	1:C:192:VAL:HG21	2.51	0.46
1:C:363:PHE:HB2	1:C:412:GLY:O	2.15	0.46
1:F:85:ASP:O	1:F:89:ALA:N	2.40	0.46
1:F:14:THR:HG23	1:F:15:SER:N	2.30	0.46
1:F:136:LYS:NZ	1:F:277:GLN:O	2.47	0.46
1:D:74:ARG:HH12	1:D:366:GLU:HG3	1.79	0.46
1:D:91:ILE:HD11	1:D:148:VAL:HG13	1.98	0.46
1:B:100:ASN:ND2	1:B:156:ARG:HH12	2.13	0.46
1:F:226:THR:OG1	1:F:226:THR:O	2.33	0.46
1:A:103:ILE:N	1:A:103:ILE:CD1	2.76	0.46
1:D:253:MET:HE3	1:D:253:MET:HB3	1.72	0.46
1:D:400:LEU:HD11	1:D:410:CYS:SG	2.56	0.46
1:B:393:LEU:O	1:B:397:LEU:HB2	2.16	0.46
1:B:200:THR:O	1:B:204:ILE:HG13	2.16	0.46
1:A:262:PRO:O	1:A:266:VAL:HG23	2.15	0.46
1:E:249:ASN:O	1:E:253:MET:HB2	2.15	0.46
1:F:362:TRP:O	1:F:410:CYS:HA	2.16	0.46
1:D:419:ILE:O	1:D:420:ASP:C	2.53	0.46
1:D:257:VAL:HG12	1:D:258:HIS:CD2	2.51	0.46
1:D:137:HIS:O	1:D:140:ASP:HB2	2.16	0.46
1:D:55:TYR:HA	1:D:98:TYR:CE1	2.50	0.46
1:B:357:TYR:O	1:B:360:ILE:HG23	2.16	0.46
1:D:54:ALA:O	1:D:58:ILE:HB	2.15	0.46
1:D:251:LEU:O	1:D:251:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HA	1:A:446:PRO:HA	1.97	0.45
1:F:188:LYS:O	1:F:192:VAL:HG23	2.16	0.45
1:E:334:ASN:ND2	1:E:337:LYS:HB2	2.31	0.45
1:B:253:MET:HE1	1:B:353:MET:CE	2.46	0.45
1:C:74:ARG:HH12	1:C:366:GLU:HG3	1.81	0.45
1:B:186:GLY:O	1:B:190:VAL:HG23	2.17	0.45
1:C:145:PHE:CE1	1:C:149:CYS:SG	3.10	0.45
1:C:259:GLY:HA3	1:C:287:ALA:HA	1.98	0.45
1:A:455:LYS:HE3	1:A:455:LYS:HB2	1.80	0.45
1:A:381:THR:O	1:A:445:ARG:NH2	2.49	0.45
1:E:433:GLY:O	1:E:447:LYS:NZ	2.45	0.45
1:C:416:TRP:CD1	1:C:417:THR:HB	2.52	0.45
1:D:378:ARG:NH2	1:D:436:GLU:OE1	2.50	0.45
1:E:114:VAL:CG1	1:E:161:PHE:HE2	2.30	0.45
1:D:100:ASN:HD22	1:D:156:ARG:HH12	1.64	0.45
1:F:197:ALA:O	1:F:200:THR:HB	2.16	0.45
1:C:50:THR:O	1:C:51:ALA:C	2.55	0.45
1:E:31:PHE:CZ	1:E:179:HIS:CD2	3.05	0.45
1:E:379:ASP:OD2	1:E:381:THR:HG22	2.16	0.45
1:E:365:SER:O	1:E:414:HIS:HB2	2.17	0.45
1:D:18:GLN:HG2	1:D:422:TRP:O	2.17	0.45
1:D:291:VAL:HB	1:D:293:TYR:O	2.17	0.45
1:E:25:LYS:NZ	1:E:32:ASP:OD2	2.48	0.45
1:B:187:LYS:HA	1:B:274:VAL:HG22	1.99	0.45
1:B:331:ARG:HG3	1:B:340:GLU:HG3	1.98	0.45
1:D:418:PRO:CD	2:D:2012:HOH:O	2.53	0.45
1:C:25:LYS:NZ	1:C:78:GLN:NE2	2.63	0.45
1:C:52:SER:O	1:C:444:ARG:NH2	2.38	0.45
1:C:180:TYR:CG	1:C:181:PRO:HA	2.52	0.45
1:B:52:SER:O	1:B:444:ARG:NH2	2.35	0.45
1:B:114:VAL:CG1	1:B:161:PHE:HE2	2.30	0.45
1:B:301:PRO:HD2	1:B:340:GLU:HB3	1.99	0.45
1:F:103:ILE:HD12	1:F:157:VAL:HG22	1.99	0.45
1:A:185:ASP:OD2	1:A:188:LYS:HD2	2.17	0.45
1:F:35:TYR:OH	1:F:45:TYR:O	2.22	0.44
1:D:312:VAL:HG23	1:D:313:ILE:H	1.81	0.44
1:D:53:ASP:HB2	1:D:442:GLN:HG3	1.98	0.44
1:F:88:GLN:O	1:F:89:ALA:HB3	2.16	0.44
1:B:270:LYS:O	1:B:272:ASP:N	2.50	0.44
1:E:56:HIS:NE2	1:F:56:HIS:CD2	2.85	0.44
1:C:23:PHE:C	1:C:25:LYS:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HD2	1:A:32:ASP:OD1	2.16	0.44
1:B:107:LEU:HD11	1:B:156:ARG:HB3	2.00	0.44
1:C:250:ASP:O	1:C:251:LEU:C	2.53	0.44
1:F:87:GLU:HA	1:F:141:LEU:HD21	1.99	0.44
1:C:171:GLU:O	1:C:172:GLY:C	2.55	0.44
1:D:100:ASN:ND2	1:D:156:ARG:HH12	2.15	0.44
1:D:234:SER:O	1:D:238:MET:HB2	2.18	0.44
1:E:225:LEU:HD21	1:E:352:LYS:CG	2.46	0.44
1:B:161:PHE:HA	1:B:220:GLY:O	2.17	0.44
1:C:375:ASP:O	1:C:378:ARG:CG	2.66	0.44
1:C:344:GLU:HG3	1:C:399:TYR:CZ	2.53	0.44
1:E:83:ILE:HG21	1:E:86:PHE:HA	2.00	0.44
1:B:9:TRP:HB2	1:B:412:GLY:HA3	1.99	0.44
1:E:120:PHE:CD1	1:E:120:PHE:N	2.84	0.44
1:B:381:THR:CG2	1:B:383:GLN:HB2	2.48	0.44
1:B:8:PHE:CE1	1:B:412:GLY:N	2.85	0.44
1:A:164:ASN:HA	1:A:222:ILE:HB	2.00	0.44
1:D:247:TRP:NE1	1:D:319:PRO:HG3	2.33	0.44
1:C:12:GLY:HA3	1:C:418:PRO:HG3	2.00	0.44
1:F:461:ARG:HE	1:F:461:ARG:HB2	1.59	0.44
1:C:300:HIS:HB2	1:C:301:PRO:HD2	2.00	0.44
1:E:285:LEU:O	1:E:289:ASN:OD1	2.36	0.44
1:D:270:LYS:O	1:D:272:ASP:N	2.50	0.44
1:D:22:ARG:HD3	1:D:49:ASP:OD1	2.17	0.44
1:F:334:ASN:HB2	1:F:341:ILE:HD11	2.00	0.44
1:D:445:ARG:O	1:D:446:PRO:C	2.56	0.44
1:F:100:ASN:HD22	1:F:100:ASN:HA	1.61	0.43
1:E:12:GLY:HA3	1:E:418:PRO:HG3	2.00	0.43
1:C:249:ASN:N	1:C:249:ASN:HD22	2.16	0.43
1:E:164:ASN:O	1:E:165:GLU:HB2	2.18	0.43
1:B:253:MET:HE3	1:B:253:MET:HB3	1.86	0.43
1:E:10:TRP:O	1:E:72:SER:OG	2.21	0.43
1:B:362:TRP:CZ2	1:B:410:CYS:HB2	2.53	0.43
1:E:226:THR:HG22	1:E:298:PHE:HD1	1.83	0.43
1:B:253:MET:CE	1:B:353:MET:HE1	2.49	0.43
1:F:297:ASN:HD21	1:F:366:GLU:HG3	1.84	0.43
1:F:299:TYR:OH	1:F:366:GLU:OE1	2.25	0.43
1:E:313:ILE:C	1:E:313:ILE:HD13	2.39	0.43
1:B:186:GLY:HA3	1:B:317:TRP:HB3	2.00	0.43
1:F:174:TYR:O	1:F:175:LEU:HD23	2.18	0.43
1:D:277:GLN:HE21	1:D:277:GLN:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASP:N	1:D:216:ASP:OD1	2.46	0.43
1:E:163:HIS:HB2	1:E:166:PRO:HD3	2.01	0.43
1:F:22:ARG:HB2	1:F:49:ASP:HA	2.00	0.43
1:B:99:TYR:HA	1:B:102:VAL:HG23	2.01	0.43
1:E:249:ASN:O	1:E:253:MET:CG	2.66	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.73	0.43
1:F:55:TYR:HD2	1:F:56:HIS:CE1	2.37	0.43
1:A:208:ARG:HH21	1:A:292:ASP:CG	2.22	0.43
1:D:248:ASN:C	1:D:249:ASN:HD22	2.21	0.43
1:F:213:GLU:CD	1:F:213:GLU:H	2.21	0.43
1:E:30:LEU:HB3	1:E:180:TYR:HB3	2.01	0.43
1:E:225:LEU:HD23	1:E:349:ILE:HG23	2.00	0.43
1:C:74:ARG:NH2	1:C:164:ASN:OD1	2.50	0.43
1:C:225:LEU:CD2	1:C:353:MET:HE2	2.48	0.43
1:A:365:SER:O	1:A:366:GLU:HG3	2.19	0.43
1:D:208:ARG:HH21	1:D:292:ASP:CG	2.21	0.43
1:B:347:TYR:O	1:B:350:ALA:HB3	2.19	0.43
1:F:78:GLN:C	1:F:80:THR:N	2.71	0.43
1:B:436:GLU:O	1:B:444:ARG:HA	2.19	0.43
1:F:437:ASN:OD1	1:F:444:ARG:NH2	2.46	0.43
1:B:127:TYR:HA	1:B:132:GLY:N	2.33	0.43
1:B:166:PRO:CB	1:B:196:LEU:HD13	2.49	0.43
1:E:363:PHE:HB2	1:E:412:GLY:O	2.19	0.42
1:B:253:MET:HE1	1:B:353:MET:HE1	2.00	0.42
1:F:87:GLU:HA	1:F:141:LEU:CD2	2.48	0.42
1:C:186:GLY:HA3	1:C:317:TRP:HB3	2.00	0.42
1:E:8:PHE:HD2	1:E:10:TRP:CE2	2.37	0.42
1:D:416:TRP:CD1	1:D:417:THR:HB	2.53	0.42
1:A:244:ALA:O	1:A:248:ASN:HB2	2.19	0.42
1:C:257:VAL:HG13	1:C:360:ILE:HD13	2.01	0.42
1:F:331:ARG:H	1:F:331:ARG:CD	2.18	0.42
1:D:294:LEU:O	1:D:362:TRP:HA	2.20	0.42
1:C:370:GLY:HA2	1:C:431:ARG:O	2.19	0.42
1:C:275:LEU:HG	1:C:276:TRP:N	2.34	0.42
1:E:274:VAL:HG22	1:E:274:VAL:O	2.19	0.42
1:C:366:GLU:HG2	1:C:416:TRP:HE3	1.84	0.42
1:B:444:ARG:HG2	1:B:444:ARG:H	1.65	0.42
1:A:218:ARG:HB3	1:A:293:TYR:CE1	2.55	0.42
1:D:456:VAL:HA	1:D:461:ARG:O	2.19	0.42
1:F:17:PRO:HD3	1:F:78:GLN:HG3	2.00	0.42
1:D:257:VAL:HG22	1:D:360:ILE:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:TRP:HA	1:B:321:TRP:CZ2	2.54	0.42
1:E:31:PHE:HZ	1:E:179:HIS:CD2	2.38	0.42
1:C:35:TYR:C	1:C:35:TYR:CD1	2.93	0.42
1:F:114:VAL:HG11	1:F:161:PHE:HE2	1.85	0.42
1:B:362:TRP:O	1:B:410:CYS:HA	2.20	0.42
1:A:112:ARG:NH2	2:A:2005:HOH:O	2.51	0.42
1:E:166:PRO:O	1:E:170:VAL:HG23	2.19	0.42
1:B:51:ALA:C	1:B:428:TYR:OH	2.58	0.42
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.89	0.42
1:B:455:LYS:O	1:B:456:VAL:C	2.58	0.42
1:A:438:ASN:OD1	1:A:438:ASN:C	2.58	0.42
1:E:14:THR:HG23	1:E:15:SER:N	2.35	0.42
1:E:103:ILE:O	1:E:106:CYS:HB2	2.20	0.42
1:B:42:PHE:O	1:B:43:TYR:C	2.58	0.42
1:F:62:LEU:HA	1:F:62:LEU:HD23	1.91	0.42
1:A:87:GLU:OE2	1:A:130:TYR:OH	2.15	0.42
1:B:314:SER:HA	1:B:315:PRO:HD2	1.92	0.42
1:F:25:LYS:HB2	1:F:81:ARG:NH1	2.35	0.42
1:B:164:ASN:HA	1:B:222:ILE:HB	2.02	0.42
1:D:352:LYS:HE3	1:D:356:HIS:CB	2.50	0.41
1:D:312:VAL:HG23	1:D:313:ILE:N	2.35	0.41
1:B:229:TYR:HB2	1:B:303:ARG:HG2	2.02	0.41
1:A:253:MET:HE1	1:A:353:MET:CE	2.50	0.41
1:F:74:ARG:HG2	1:F:75:THR:N	2.35	0.41
1:F:343:PRO:HG3	1:F:395:GLU:OE1	2.20	0.41
1:E:133:TRP:HB3	1:E:192:VAL:HG13	2.02	0.41
1:B:253:MET:HE2	1:B:353:MET:CE	2.50	0.41
1:F:12:GLY:HA2	1:F:415:VAL:O	2.21	0.41
1:A:180:TYR:CG	1:A:181:PRO:HA	2.55	0.41
1:D:263:GLU:H	1:D:263:GLU:HG2	1.64	0.41
1:D:33:TYR:CD2	1:D:124:ILE:HG12	2.55	0.41
1:C:92:ASN:HA	1:C:93:PRO:HD3	1.93	0.41
1:D:397:LEU:HD13	1:D:413:TYR:CD1	2.55	0.41
1:E:419:ILE:O	1:E:420:ASP:C	2.58	0.41
1:F:291:VAL:HG21	1:F:294:LEU:HD21	2.02	0.41
1:A:291:VAL:HB	1:A:293:TYR:O	2.20	0.41
1:D:198:LEU:O	1:D:202:LYS:HG3	2.20	0.41
1:A:16:GLY:N	1:A:17:PRO:CD	2.84	0.41
1:F:83:ILE:HG21	1:F:86:PHE:HA	2.02	0.41
1:C:62:LEU:HD23	1:C:62:LEU:HA	1.85	0.41
1:A:419:ILE:O	1:A:420:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:MET:HA	1:E:329:PRO:HD2	1.90	0.41
1:D:136:LYS:HZ1	1:D:194:TYR:HE2	1.69	0.41
1:F:180:TYR:CD1	1:F:181:PRO:HA	2.55	0.41
1:B:100:ASN:ND2	1:B:156:ARG:HH22	2.18	0.41
1:C:15:SER:HB3	1:C:119:HIS:CD2	2.56	0.41
1:A:42:PHE:CD1	1:A:42:PHE:N	2.88	0.41
1:E:37:GLU:C	1:E:38:GLU:HG3	2.40	0.41
1:C:225:LEU:CD2	1:C:353:MET:CE	2.97	0.41
1:E:54:ALA:O	1:E:98:TYR:OH	2.35	0.41
1:E:363:PHE:HE2	1:E:414:HIS:ND1	2.18	0.41
1:A:74:ARG:HH12	1:A:366:GLU:HG3	1.86	0.41
1:E:116:ASN:HA	1:E:161:PHE:O	2.21	0.41
1:D:173:SER:N	1:D:179:HIS:HB2	2.35	0.41
1:B:190:VAL:HG21	1:B:274:VAL:HG13	2.02	0.41
1:A:5:PRO:HD2	1:A:8:PHE:CD1	2.56	0.41
1:B:328:MET:O	1:B:331:ARG:CD	2.67	0.41
1:D:74:ARG:NH1	1:D:366:GLU:HG3	2.36	0.41
1:F:337:LYS:HG2	1:F:339:TRP:CE3	2.56	0.41
1:F:298:PHE:HE2	1:F:396:HIS:CD2	2.38	0.41
1:A:243:PHE:CD2	1:A:322:TYR:HB2	2.55	0.41
1:F:263:GLU:HG2	1:F:263:GLU:H	1.62	0.41
1:C:120:PHE:CD1	1:C:120:PHE:N	2.89	0.41
1:B:277:GLN:HE21	1:B:277:GLN:N	2.19	0.41
1:B:66:ALA:HB2	1:B:109:ASN:HB3	2.02	0.41
1:E:207:TYR:O	1:E:215:SER:CB	2.67	0.41
1:F:91:ILE:HG22	1:F:92:ASN:N	2.36	0.41
1:C:444:ARG:HG2	1:C:444:ARG:H	1.37	0.41
1:C:433:GLY:O	1:C:447:LYS:NZ	2.48	0.41
1:E:389:ARG:NH2	1:E:431:ARG:O	2.54	0.41
1:A:257:VAL:HG12	1:A:258:HIS:CD2	2.55	0.40
1:F:186:GLY:O	1:F:187:LYS:C	2.60	0.40
1:F:65:LEU:O	1:F:68:LEU:N	2.54	0.40
1:C:161:PHE:HA	1:C:220:GLY:O	2.21	0.40
1:A:313:ILE:HD13	1:A:313:ILE:HA	1.92	0.40
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.90	0.40
1:C:57:GLN:O	1:C:58:ILE:C	2.59	0.40
1:F:223:LEU:HB3	1:F:224:ASN:H	1.80	0.40
1:C:29:ASN:ND2	1:C:78:GLN:NE2	2.68	0.40
1:D:127:TYR:HA	1:D:132:GLY:N	2.36	0.40
1:E:369:VAL:O	1:E:389:ARG:NH2	2.50	0.40
1:D:186:GLY:HA3	1:D:317:TRP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ASP:C	1:E:55:TYR:N	2.75	0.40
1:D:438:ASN:O	1:D:442:GLN:N	2.53	0.40
1:E:187:LYS:HA	1:E:274:VAL:CG2	2.51	0.40
1:E:123:PRO:HD2	1:E:126:LEU:HD12	2.02	0.40
1:E:127:TYR:HA	1:E:132:GLY:N	2.36	0.40
1:E:436:GLU:O	1:E:444:ARG:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/479 (96%)	423 (92%)	32 (7%)	4 (1%)	21	42
1	B	459/479 (96%)	420 (92%)	34 (7%)	5 (1%)	17	36
1	C	459/479 (96%)	420 (92%)	37 (8%)	2 (0%)	39	65
1	D	459/479 (96%)	416 (91%)	38 (8%)	5 (1%)	17	36
1	E	459/479 (96%)	404 (88%)	51 (11%)	4 (1%)	21	42
1	F	459/479 (96%)	408 (89%)	47 (10%)	4 (1%)	21	42
All	All	2754/2874 (96%)	2491 (90%)	239 (9%)	24 (1%)	21	42

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	24	ALA
1	B	271	LYS
1	D	209	ARG
1	E	344	GLU
1	F	24	ALA
1	F	336	ASP

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Mol	Chain	Res	Type
1	B	7	GLU
1	B	420	ASP
1	C	24	ALA
1	D	51	ALA
1	D	271	LYS
1	E	23	PHE
1	F	358	ASP
1	A	51	ALA
1	A	375	ASP
1	A	380	GLU
1	B	24	ALA
1	F	23	PHE
1	A	336	ASP
1	D	358	ASP
1	B	456	VAL
1	D	446	PRO
1	E	279	THR
1	C	315	PRO

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	389/404 (96%)	365 (94%)	24 (6%)	23 45
1	B	389/404 (96%)	371 (95%)	18 (5%)	33 61
1	C	389/404 (96%)	364 (94%)	25 (6%)	22 43
1	D	389/404 (96%)	367 (94%)	22 (6%)	25 49
1	E	389/404 (96%)	372 (96%)	17 (4%)	35 63
1	F	389/404 (96%)	365 (94%)	24 (6%)	23 45
All	All	2334/2424 (96%)	2204 (94%)	130 (6%)	26 50

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	103	ILE
1	A	135	SER
1	A	146	SER
1	A	155	ASP
1	A	176	MET
1	A	218	ARG
1	A	260	LYS
1	A	276	TRP
1	A	277	GLN
1	A	279	THR
1	A	293	TYR
1	A	313	ILE
1	A	314	SER
1	A	327	LEU
1	A	331	ARG
1	A	336	ASP
1	A	359	ASN
1	A	363	PHE
1	A	378	ARG
1	A	397	LEU
1	A	423	SER
1	A	444	ARG
1	A	445	ARG
1	B	2	LEU
1	B	67	SER
1	B	135	SER
1	B	226	THR
1	B	233	GLN
1	B	274	VAL
1	B	277	GLN
1	B	279	THR
1	B	293	TYR
1	B	302	LYS
1	B	313	ILE
1	B	331	ARG
1	B	378	ARG
1	B	383	GLN
1	B	397	LEU
1	B	405	GLU
1	B	444	ARG
1	B	445	ARG
1	C	40	ASP

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Mol	Chain	Res	Type
1	C	67	SER
1	C	75	THR
1	C	135	SER
1	C	155	ASP
1	C	204	ILE
1	C	214	LEU
1	C	226	THR
1	C	238	MET
1	C	263	GLU
1	C	274	VAL
1	C	276	TRP
1	C	277	GLN
1	C	279	THR
1	C	293	TYR
1	C	313	ILE
1	C	331	ARG
1	C	336	ASP
1	C	359	ASN
1	C	365	SER
1	C	378	ARG
1	C	380	GLU
1	C	397	LEU
1	C	444	ARG
1	C	445	ARG
1	D	6	LYS
1	D	44	ASP
1	D	74	ARG
1	D	135	SER
1	D	226	THR
1	D	238	MET
1	D	263	GLU
1	D	277	GLN
1	D	279	THR
1	D	293	TYR
1	D	311	PRO
1	D	313	ILE
1	D	314	SER
1	D	327	LEU
1	D	331	ARG
1	D	359	ASN
1	D	378	ARG
1	D	380	GLU

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Mol	Chain	Res	Type
1	D	397	LEU
1	D	423	SER
1	D	444	ARG
1	D	445	ARG
1	E	2	LEU
1	E	7	GLU
1	E	44	ASP
1	E	147	LYS
1	E	226	THR
1	E	227	PRO
1	E	260	LYS
1	E	277	GLN
1	E	279	THR
1	E	293	TYR
1	E	313	ILE
1	E	327	LEU
1	E	331	ARG
1	E	365	SER
1	E	444	ARG
1	E	445	ARG
1	E	462	LEU
1	F	7	GLU
1	F	17	PRO
1	F	146	SER
1	F	225	LEU
1	F	260	LYS
1	F	274	VAL
1	F	276	TRP
1	F	277	GLN
1	F	283	LEU
1	F	293	TYR
1	F	313	ILE
1	F	327	LEU
1	F	331	ARG
1	F	333	MET
1	F	336	ASP
1	F	363	PHE
1	F	365	SER
1	F	376	ARG
1	F	378	ARG
1	F	380	GLU
1	F	423	SER

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Mol	Chain	Res	Type
1	F	444	ARG
1	F	445	ARG
1	F	462	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	78	GLN
1	A	100	ASN
1	A	119	HIS
1	A	152	GLN
1	A	248	ASN
1	A	249	ASN
1	A	258	HIS
1	A	277	GLN
1	A	289	ASN
1	A	297	ASN
1	A	359	ASN
1	A	367	ASN
1	A	383	GLN
1	A	426	ASN
1	A	430	ASN
1	B	56	HIS
1	B	57	GLN
1	B	78	GLN
1	B	100	ASN
1	B	249	ASN
1	B	258	HIS
1	B	277	GLN
1	B	289	ASN
1	B	297	ASN
1	B	359	ASN
1	C	18	GLN
1	C	56	HIS
1	C	78	GLN
1	C	100	ASN
1	C	119	HIS
1	C	152	GLN
1	C	248	ASN
1	C	249	ASN
1	C	277	GLN

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Mol	Chain	Res	Type
1	C	289	ASN
1	C	359	ASN
1	C	367	ASN
1	C	383	GLN
1	C	430	ASN
1	D	56	HIS
1	D	57	GLN
1	D	78	GLN
1	D	100	ASN
1	D	233	GLN
1	D	249	ASN
1	D	258	HIS
1	D	277	GLN
1	D	297	ASN
1	D	359	ASN
1	D	385	GLN
1	D	459	HIS
1	E	56	HIS
1	E	78	GLN
1	E	100	ASN
1	E	119	HIS
1	E	179	HIS
1	E	249	ASN
1	E	289	ASN
1	E	297	ASN
1	E	359	ASN
1	E	367	ASN
1	E	385	GLN
1	E	430	ASN
1	F	56	HIS
1	F	57	GLN
1	F	78	GLN
1	F	100	ASN
1	F	179	HIS
1	F	233	GLN
1	F	289	ASN
1	F	297	ASN
1	F	359	ASN
1	F	367	ASN
1	F	414	HIS
1	F	426	ASN
1	F	430	ASN

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Mol	Chain	Res	Type
1	F	459	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	461/479 (96%)	-0.40	0 100 100	17, 32, 49, 65	1 (0%)
1	B	461/479 (96%)	-0.36	2 (0%) 93 91	16, 31, 50, 68	1 (0%)
1	C	461/479 (96%)	-0.36	0 100 100	21, 36, 56, 81	1 (0%)
1	D	461/479 (96%)	-0.39	0 100 100	19, 34, 56, 70	1 (0%)
1	E	461/479 (96%)	-0.16	1 (0%) 95 95	23, 46, 65, 89	1 (0%)
1	F	461/479 (96%)	-0.08	3 (0%) 89 87	28, 49, 74, 91	1 (0%)
All	All	2766/2874 (96%)	-0.29	6 (0%) 95 95	16, 38, 62, 91	6 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	225	LEU	3.4
1	F	273	GLY	3.1
1	B	315	PRO	2.3
1	F	286	ILE	2.1
1	E	273	GLY	2.1
1	B	312	VAL	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.