Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:39 PM GMT

PDB ID	:	4M4R
Title	:	Epha4 ectodomain complex with ephrin a5
Authors	:	Xu, K.; Tsvetkova-Robev, D.; Xu, Y.; Goldgur, Y.; Chan, Y.-P.; Himanen, J.P.; Nikolov, D.B.
Deposited on	:	2013-08-07
Resolution	:	3.13 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:

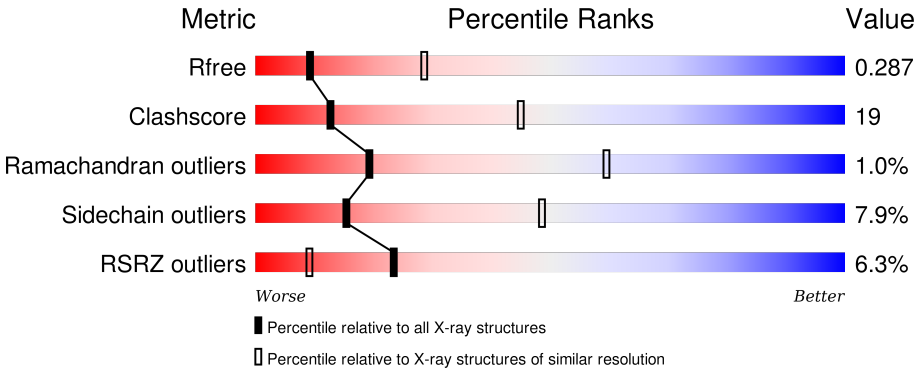
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.13 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	518	8% 71% 26%
1	C	518	5% 69% 27%
1	E	518	9% 72% 23%
1	G	518	8% 68% 28%
2	B	141	% 64% 32%

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Mol	Chain	Length	Quality of chain
2	D	141	2% 58% 36%
2	F	141	% 52% 40% 5%
2	H	141	6% 48% 42% 7%

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
4	NAG	C	601	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20947 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 Ephrin type-A receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4014	2502	694	792	26			
1	C	516	Total	C	N	O	S	0	0	0
			4014	2502	694	792	26			
1	E	516	Total	C	N	O	S	0	0	0
			4014	2502	694	792	26			
1	G	516	Total	C	N	O	S	0	0	0
			4014	2502	694	792	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	EXPRESSION TAG	UNP P54764
C	26	ALA	-	EXPRESSION TAG	UNP P54764
E	26	ALA	-	EXPRESSION TAG	UNP P54764
G	26	ALA	-	EXPRESSION TAG	UNP P54764

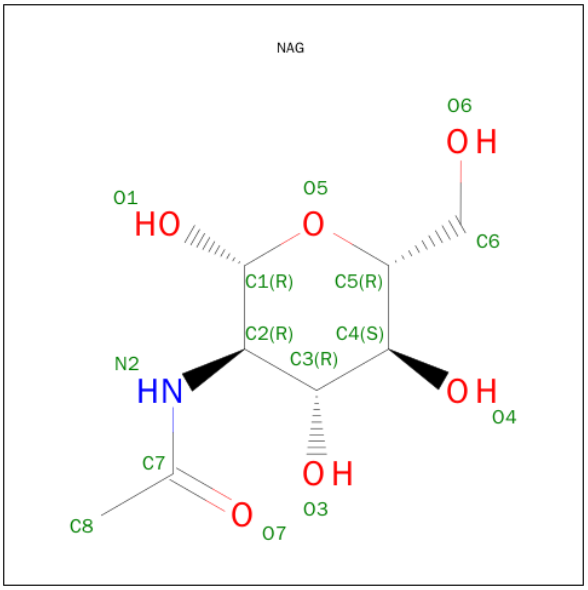
- Molecule 2 is a protein called Ephrin-A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1165	745	201	211	8			
2	D	140	Total	C	N	O	S	0	0	0
			1160	742	200	210	8			
2	F	138	Total	C	N	O	S	0	0	0
			1150	736	198	208	8			
2	H	138	Total	C	N	O	S	0	0	0
			1150	736	198	208	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ALA	-	EXPRESSION TAG	UNP P52803
B	26	ALA	-	EXPRESSION TAG	UNP P52803
D	25	ALA	-	EXPRESSION TAG	UNP P52803
D	26	ALA	-	EXPRESSION TAG	UNP P52803
F	25	ALA	-	EXPRESSION TAG	UNP P52803
F	26	ALA	-	EXPRESSION TAG	UNP P52803
H	25	ALA	-	EXPRESSION TAG	UNP P52803
H	26	ALA	-	EXPRESSION TAG	UNP P52803

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

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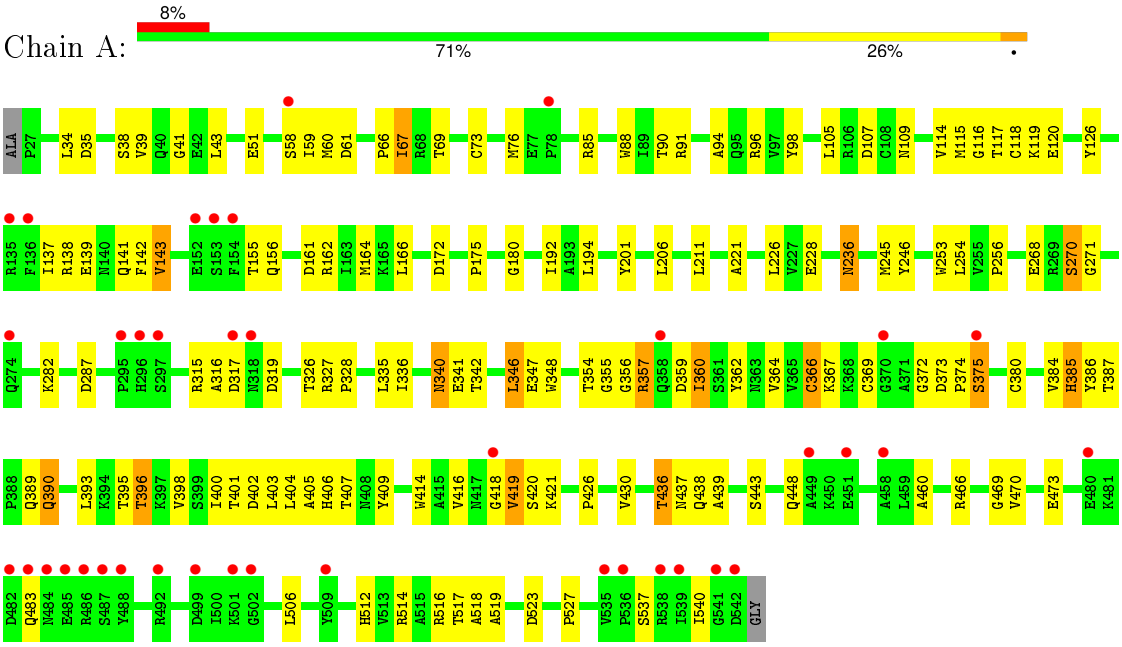
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

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.

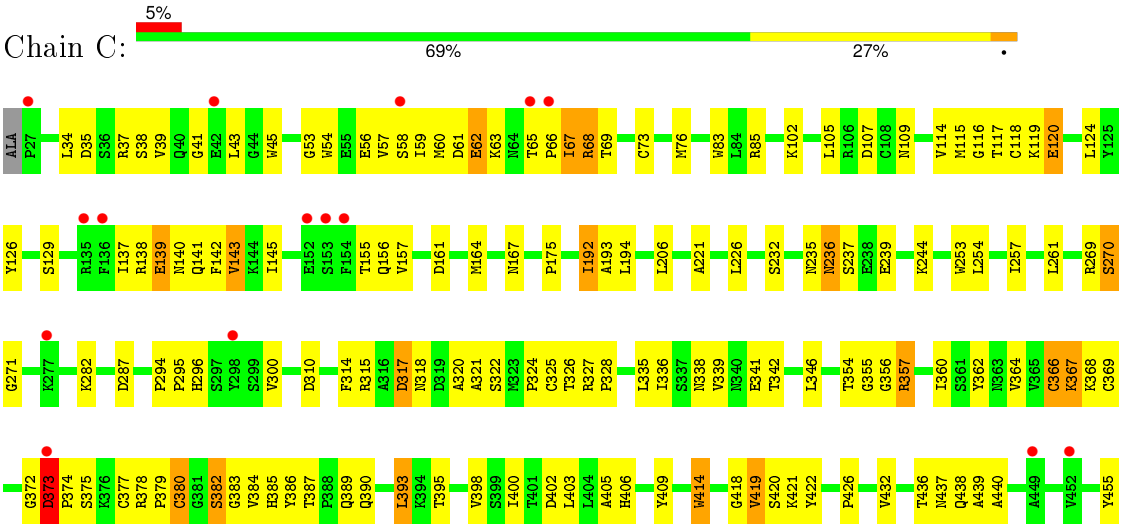
- Molecule 1: Ephrin type-A receptor 4

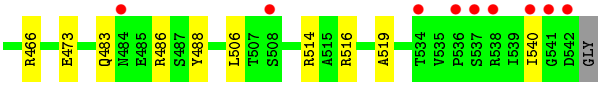
Chain A:



- Molecule 1: Ephrin type-A receptor 4

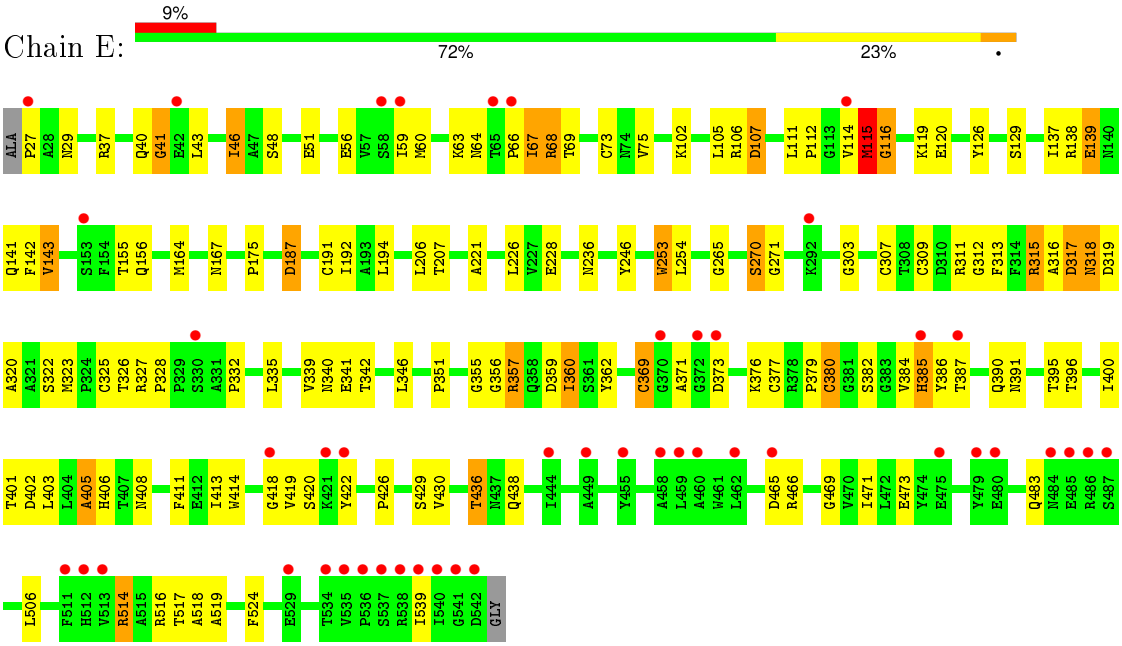
Chain C:





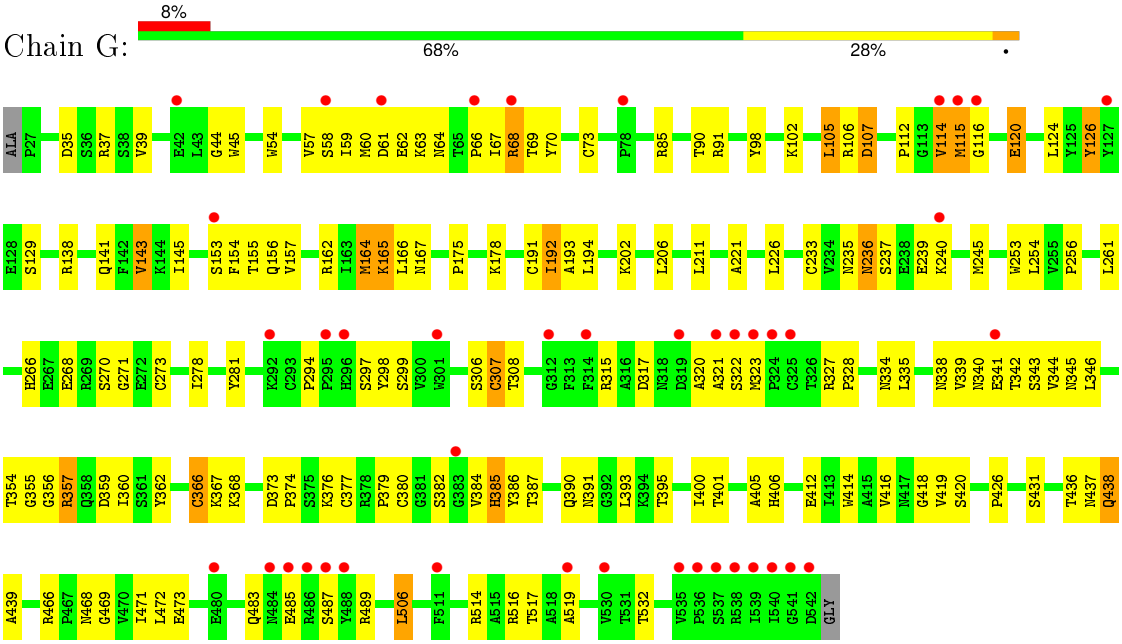
• Molecule 1: Ephrin type-A receptor 4

Chain E:



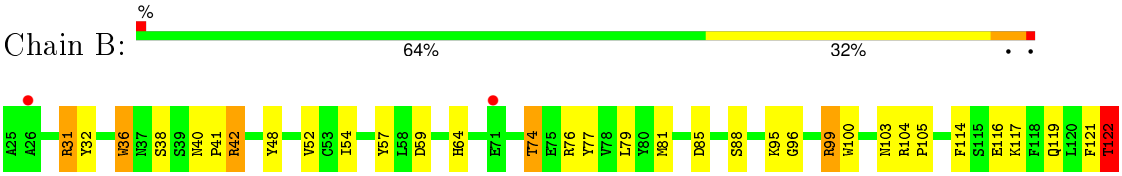
• Molecule 1: Ephrin type-A receptor 4

Chain G:



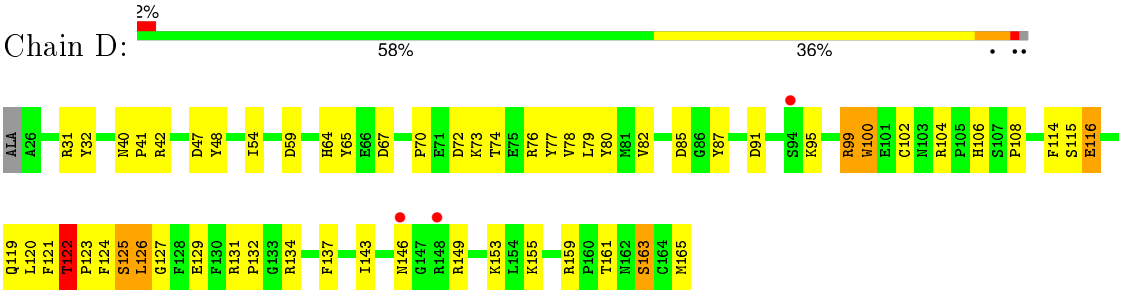
• Molecule 2: Ephrin-A5

Chain B:



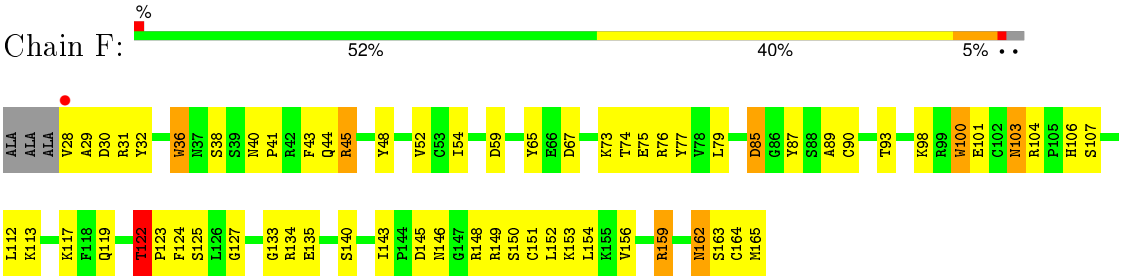
• Molecule 2: Ephrin-A5

Chain D:



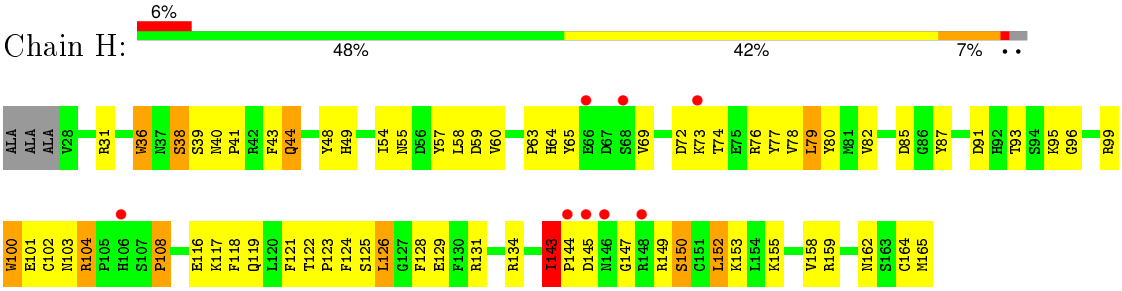
• Molecule 2: Ephrin-A5

Chain F:



• Molecule 2: Ephrin-A5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	207.54Å 46.69Å 262.31Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	30.00 – 3.13 29.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.13) 99.4 (29.80-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.244 , 0.290 0.241 , 0.287	Depositor DCC
R_{free} test set	4496 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 87.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 92122 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20947	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

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

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	0.66	1/4100 (0.0%)	0.78	1/5579 (0.0%)
1	C	0.75	4/4100 (0.1%)	0.86	2/5579 (0.0%)
1	E	0.63	1/4100 (0.0%)	0.80	7/5579 (0.1%)
1	G	0.58	2/4100 (0.0%)	0.73	2/5579 (0.0%)
2	B	0.90	2/1204 (0.2%)	0.94	2/1631 (0.1%)
2	D	0.93	2/1199 (0.2%)	0.94	3/1624 (0.2%)
2	F	0.76	2/1189 (0.2%)	0.85	1/1610 (0.1%)
2	H	0.68	2/1189 (0.2%)	0.78	2/1610 (0.1%)
All	All	0.70	16/21181 (0.1%)	0.81	20/28791 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	H	0	1
4	C	1	0
All	All	1	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	116	GLU	CD-OE1	6.82	1.33	1.25
1	C	414	TRP	CD2-CE2	6.66	1.49	1.41
1	C	54	TRP	CD2-CE2	6.56	1.49	1.41
2	D	100	TRP	CD2-CE2	6.55	1.49	1.41
1	A	253	TRP	CD2-CE2	6.09	1.48	1.41
1	C	253	TRP	CD2-CE2	6.04	1.48	1.41
2	H	100	TRP	CD2-CE2	5.85	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	253	TRP	CD2-CE2	5.84	1.48	1.41
1	G	54	TRP	CD2-CE2	5.79	1.48	1.41
2	B	100	TRP	CD2-CE2	5.70	1.48	1.41
2	H	36	TRP	CD2-CE2	5.69	1.48	1.41
2	F	100	TRP	CD2-CE2	5.67	1.48	1.41
2	F	36	TRP	CD2-CE2	5.61	1.48	1.41
1	E	253	TRP	CD2-CE2	5.57	1.48	1.41
1	C	83	TRP	CD2-CE2	5.12	1.47	1.41
2	B	36	TRP	CD2-CE2	5.02	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	126	LEU	CB-CG-CD1	-7.69	97.92	111.00
1	E	115	MET	CG-SD-CE	7.47	112.15	100.20
1	E	115	MET	CA-CB-CG	6.52	124.39	113.30
2	D	99	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	161	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	H	143	ILE	CB-CA-C	6.29	124.19	111.60
1	E	187	ASP	CB-CG-OD2	6.17	123.85	118.30
2	B	122	THR	CB-CA-C	-6.06	95.24	111.60
2	F	122	THR	CB-CA-C	-6.06	95.25	111.60
1	A	91	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	E	68	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	E	107	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	67	ILE	CB-CA-C	-5.20	101.20	111.60
1	G	44	GLY	N-CA-C	-5.19	100.12	113.10
1	C	53	GLY	N-CA-C	-5.19	100.14	113.10
2	D	122	THR	CB-CA-C	-5.15	97.70	111.60
1	G	114	VAL	N-CA-C	5.13	124.84	111.00
2	D	126	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	E	68	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	99	ARG	CG-CD-NE	-5.00	101.29	111.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	601	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	116	GLY	Peptide
2	H	143	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4014	0	3868	169	0
1	C	4014	0	3873	175	0
1	E	4014	0	3870	148	1
1	G	4014	0	3870	187	1
2	B	1165	0	1082	45	0
2	D	1160	0	1077	38	0
2	F	1150	0	1067	53	0
2	H	1150	0	1067	62	0
3	A	14	0	13	0	0
3	E	14	0	12	0	0
3	G	14	0	13	0	0
4	A	28	0	23	0	0
4	B	28	0	25	1	0
4	C	28	0	25	0	0
4	D	28	0	25	1	0
4	E	28	0	25	3	0
4	F	28	0	25	0	0
4	G	28	0	25	1	0
4	H	28	0	25	3	0
All	All	20947	0	20010	788	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (788) 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:A:406:HIS:CE1	1:A:438:GLN:HB3	1.53	1.40
1:A:406:HIS:HE1	1:A:438:GLN:CB	1.47	1.28
1:C:372:GLY:C	1:C:374:PRO:HD3	1.54	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:PRO:HG3	1:G:322:SER:O	1.31	1.24
1:C:117:THR:N	1:G:115:MET:SD	2.11	1.24
1:G:299:SER:N	1:G:307:CYS:SG	2.10	1.24
1:A:341:GLU:HA	1:A:437:ASN:CB	1.69	1.22
1:G:294:PRO:CG	1:G:322:SER:O	1.89	1.19
1:A:60:MET:CE	1:A:66:PRO:HA	1.75	1.17
1:G:385:HIS:HA	1:G:386:TYR:HB2	1.26	1.16
1:A:114:VAL:O	1:E:115:MET:CB	1.93	1.16
2:H:143:ILE:HG23	2:H:144:PRO:CD	1.76	1.15
1:G:298:TYR:C	1:G:307:CYS:SG	2.25	1.14
1:G:298:TYR:HA	1:G:307:CYS:SG	1.88	1.13
1:C:118:CYS:HB3	1:G:115:MET:HE3	1.15	1.12
1:A:341:GLU:CA	1:A:437:ASN:HB3	1.78	1.12
1:G:294:PRO:HG3	1:G:322:SER:C	1.70	1.11
1:A:115:MET:CA	1:E:115:MET:HB2	1.78	1.11
1:C:57:VAL:HG13	1:C:59:ILE:CD1	1.81	1.11
1:C:118:CYS:CB	1:G:115:MET:HE3	1.81	1.10
1:E:385:HIS:HA	1:E:386:TYR:HB2	1.32	1.10
1:A:60:MET:HE1	1:A:66:PRO:CA	1.80	1.10
2:H:143:ILE:HG23	2:H:144:PRO:HD3	1.33	1.09
1:A:73:CYS:HB2	2:B:123:PRO:HG3	1.35	1.09
1:C:115:MET:HE2	1:G:114:VAL:HA	1.27	1.08
1:G:298:TYR:CA	1:G:307:CYS:SG	2.41	1.08
1:C:372:GLY:O	1:C:374:PRO:CD	2.03	1.07
1:A:116:GLY:N	1:E:115:MET:SD	2.27	1.07
1:C:73:CYS:HB2	2:D:123:PRO:HG3	1.33	1.07
1:A:335:LEU:CD1	1:A:346:LEU:HD21	1.84	1.06
2:B:74:THR:HG22	2:B:76:ARG:HH11	1.14	1.06
1:C:295:PRO:HG2	1:C:324:PRO:HB3	1.37	1.06
1:A:60:MET:HE3	1:A:66:PRO:HB3	1.36	1.05
1:A:115:MET:C	1:E:115:MET:SD	2.34	1.05
1:G:335:LEU:HD11	1:G:346:LEU:HD21	1.35	1.05
1:A:114:VAL:O	1:E:115:MET:CG	2.05	1.05
1:G:294:PRO:HG3	1:G:322:SER:CA	1.89	1.03
1:A:342:THR:CG2	1:A:403:LEU:O	2.08	1.02
1:A:342:THR:HG23	1:A:403:LEU:O	1.57	1.01
1:A:373:ASP:N	1:A:374:PRO:HD2	1.75	1.01
1:A:385:HIS:HA	1:A:386:TYR:HB2	1.41	1.01
1:C:118:CYS:CB	1:G:115:MET:CE	2.37	1.01
1:A:115:MET:HA	1:E:115:MET:HB2	1.05	1.01
1:A:341:GLU:HA	1:A:437:ASN:HB3	1.03	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG13	1:C:59:ILE:HD12	1.41	1.00
1:A:335:LEU:HD11	1:A:346:LEU:HD21	1.42	1.00
1:A:115:MET:HA	1:E:115:MET:CB	1.92	0.99
1:A:118:CYS:H	1:E:115:MET:HG2	1.27	0.99
1:G:281:TYR:OH	1:G:322:SER:HB2	1.62	0.99
1:C:372:GLY:O	1:C:374:PRO:HD2	1.59	0.97
1:C:372:GLY:C	1:C:374:PRO:CD	2.32	0.97
1:A:406:HIS:CE1	1:A:469:GLY:HA2	1.99	0.96
1:G:405:ALA:O	1:G:436:THR:HB	1.63	0.96
1:C:39:VAL:CG1	1:C:43:LEU:HB2	1.94	0.96
1:C:118:CYS:HB3	1:G:115:MET:CE	1.94	0.96
1:C:118:CYS:H	1:G:115:MET:CE	1.79	0.95
1:G:338:ASN:HB3	1:G:345:ASN:HB2	1.49	0.94
2:H:64:HIS:H	4:H:201:NAG:H81	1.33	0.94
1:E:342:THR:HG21	1:E:403:LEU:O	1.69	0.93
1:A:116:GLY:H	1:E:115:MET:H	1.11	0.92
1:E:342:THR:CG2	1:E:403:LEU:O	2.18	0.92
1:E:59:ILE:HG22	1:E:60:MET:N	1.85	0.92
1:G:335:LEU:CD1	1:G:346:LEU:HD21	1.99	0.91
2:B:122:THR:HG22	2:B:124:PHE:H	1.34	0.91
1:A:60:MET:HE1	1:A:66:PRO:HA	0.92	0.91
1:C:58:SER:O	1:C:59:ILE:HG13	1.69	0.90
2:H:143:ILE:CG2	2:H:144:PRO:HD2	2.02	0.90
1:A:406:HIS:CE1	1:A:438:GLN:CB	2.33	0.90
2:H:143:ILE:CG2	2:H:144:PRO:CD	2.49	0.89
1:E:405:ALA:O	1:E:436:THR:HB	1.72	0.88
1:A:60:MET:CE	1:A:66:PRO:CA	2.45	0.88
1:A:114:VAL:O	1:E:115:MET:HB3	1.74	0.87
2:D:122:THR:HG21	2:D:127:GLY:HA3	1.56	0.87
1:G:294:PRO:HG3	1:G:322:SER:HA	1.55	0.86
1:C:118:CYS:HB2	1:G:115:MET:HE1	1.56	0.86
1:E:59:ILE:CG2	1:E:60:MET:N	2.36	0.86
1:C:295:PRO:CG	1:C:324:PRO:HB3	2.05	0.85
1:C:39:VAL:HG11	1:C:43:LEU:HB2	1.55	0.85
1:C:155:THR:HG22	1:C:156:GLN:N	1.90	0.85
1:C:57:VAL:HG13	1:C:59:ILE:HD11	1.55	0.85
1:E:67:ILE:HG22	1:E:68:ARG:N	1.89	0.85
1:A:406:HIS:CE1	1:A:469:GLY:CA	2.59	0.84
1:C:372:GLY:O	1:C:374:PRO:HD3	1.72	0.84
1:C:254:LEU:HD13	1:G:226:LEU:HD12	1.57	0.84
1:E:335:LEU:CD1	1:E:346:LEU:HD21	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HE3	1:A:66:PRO:CB	2.08	0.83
1:A:341:GLU:HA	1:A:437:ASN:CG	1.98	0.83
1:A:116:GLY:H	1:E:115:MET:N	1.76	0.83
1:A:114:VAL:O	1:E:115:MET:HB2	1.78	0.83
1:E:155:THR:HG22	1:E:156:GLN:N	1.94	0.82
2:B:74:THR:HG22	2:B:76:ARG:NH1	1.95	0.82
1:C:385:HIS:HA	1:C:386:TYR:HB2	1.61	0.82
1:C:335:LEU:HD11	1:C:346:LEU:HD21	1.62	0.82
1:G:344:VAL:HB	1:G:400:ILE:HB	1.63	0.81
1:G:335:LEU:HD11	1:G:346:LEU:CD2	2.09	0.80
2:H:64:HIS:N	4:H:201:NAG:H81	1.95	0.80
1:C:118:CYS:HB2	1:G:115:MET:CE	2.11	0.80
2:H:119:GLN:NE2	2:H:122:THR:HG22	1.97	0.80
1:G:155:THR:HG22	1:G:156:GLN:H	1.46	0.79
1:C:254:LEU:HD13	1:G:226:LEU:CD1	2.12	0.79
2:B:122:THR:HG21	2:B:127:GLY:HA3	1.65	0.78
2:F:122:THR:HG22	2:F:124:PHE:H	1.46	0.78
2:H:76:ARG:HG2	2:H:103:ASN:HA	1.65	0.78
1:A:116:GLY:N	1:E:115:MET:H	1.82	0.78
1:C:116:GLY:H	1:G:115:MET:H	1.31	0.78
1:A:406:HIS:HE1	1:A:438:GLN:HB2	1.45	0.77
1:C:57:VAL:CG1	1:C:59:ILE:HD11	2.14	0.77
1:E:342:THR:O	1:E:342:THR:HG22	1.84	0.77
1:C:57:VAL:CG1	1:C:59:ILE:CD1	2.62	0.77
2:B:148:ARG:HB3	2:B:150:SER:O	1.83	0.77
1:A:373:ASP:N	1:A:374:PRO:CD	2.48	0.76
1:C:37:ARG:NH1	1:C:62:GLU:OE2	2.17	0.76
1:G:155:THR:HG22	1:G:156:GLN:N	2.00	0.76
1:A:35:ASP:HB3	1:A:38:SER:HB3	1.67	0.76
1:G:298:TYR:O	1:G:308:THR:N	2.19	0.76
1:C:382:SER:OG	1:C:384:VAL:HG13	1.85	0.75
1:C:114:VAL:O	1:G:115:MET:SD	2.45	0.75
1:G:294:PRO:CG	1:G:322:SER:HA	2.16	0.75
1:C:294:PRO:HG2	1:C:315:ARG:HH11	1.52	0.74
1:A:60:MET:CE	1:A:66:PRO:HB3	2.17	0.74
1:E:155:THR:HG22	1:E:156:GLN:H	1.51	0.74
1:C:373:ASP:N	1:C:374:PRO:HD3	2.01	0.73
2:H:76:ARG:HH21	2:H:143:ILE:HG21	1.53	0.73
1:C:438:GLN:O	1:C:519:ALA:HB2	1.87	0.73
1:E:46:ILE:N	1:E:46:ILE:HD13	2.02	0.73
1:G:385:HIS:CA	1:G:386:TYR:HB2	2.13	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:ALA:HB2	4:E:3402:NAG:C6	2.18	0.73
1:C:116:GLY:N	1:G:115:MET:SD	2.61	0.73
2:H:143:ILE:HG22	2:H:144:PRO:HD2	1.70	0.73
1:A:389:GLN:HB2	1:A:393:LEU:HD13	1.71	0.73
1:A:116:GLY:N	1:E:115:MET:CG	2.52	0.72
1:A:270:SER:OG	1:A:271:GLY:N	2.21	0.72
1:A:155:THR:HG22	1:A:156:GLN:N	2.04	0.72
1:C:270:SER:OG	1:C:271:GLY:N	2.22	0.72
1:A:438:GLN:HE21	1:A:518:ALA:HB3	1.54	0.72
1:G:379:PRO:O	1:G:380:CYS:SG	2.48	0.72
2:H:76:ARG:NH2	2:H:143:ILE:HG21	2.05	0.72
1:G:226:LEU:HD21	1:G:254:LEU:HD12	1.70	0.71
1:G:61:ASP:OD2	1:G:67:ILE:HD12	1.91	0.71
1:E:315:ARG:HD3	1:E:323:MET:O	1.91	0.71
2:B:42:ARG:NH1	2:B:42:ARG:HB3	2.06	0.71
1:A:85:ARG:HD3	1:A:137:ILE:HG12	1.73	0.70
2:B:99:ARG:NH2	2:B:116:GLU:OE1	2.23	0.70
1:G:294:PRO:CD	1:G:322:SER:HA	2.22	0.70
1:C:116:GLY:C	1:G:115:MET:SD	2.70	0.70
1:A:35:ASP:O	1:A:39:VAL:HG23	1.92	0.70
1:A:406:HIS:ND1	1:A:469:GLY:HA2	2.06	0.69
1:E:438:GLN:NE2	1:E:518:ALA:HB3	2.06	0.69
2:D:122:THR:HG22	2:D:124:PHE:H	1.58	0.69
2:H:87:TYR:CE1	2:H:153:LYS:HB3	2.28	0.69
1:E:473:GLU:OE1	1:E:516:ARG:NH1	2.24	0.69
1:C:341:GLU:O	1:C:436:THR:CG2	2.41	0.69
1:G:59:ILE:HG22	1:G:60:MET:N	2.08	0.69
1:C:341:GLU:O	1:C:436:THR:HG23	1.93	0.68
1:C:155:THR:CG2	1:C:156:GLN:N	2.56	0.68
1:C:335:LEU:HD21	1:C:432:VAL:HG12	1.75	0.68
1:A:342:THR:HG22	1:A:342:THR:O	1.94	0.67
1:C:328:PRO:HB3	1:C:420:SER:CB	2.24	0.67
2:F:28:VAL:HG12	2:F:29:ALA:N	2.09	0.67
1:C:118:CYS:N	1:G:115:MET:CE	2.55	0.67
1:A:405:ALA:O	1:A:436:THR:HB	1.94	0.67
2:B:121:PHE:HA	2:B:129:GLU:OE2	1.95	0.67
2:F:41:PRO:O	2:F:44:GLN:HB2	1.95	0.67
1:E:438:GLN:O	1:E:519:ALA:HB2	1.95	0.67
1:A:439:ALA:HA	1:A:519:ALA:CB	2.25	0.67
1:A:114:VAL:O	1:E:115:MET:HG2	1.95	0.66
1:A:385:HIS:O	1:A:401:THR:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:CYS:HB2	2:F:123:PRO:HG3	1.75	0.66
1:E:46:ILE:CD1	1:E:46:ILE:N	2.57	0.66
1:G:107:ASP:OD1	1:G:153:SER:OG	2.11	0.66
2:B:42:ARG:HB3	2:B:42:ARG:HH11	1.60	0.66
1:A:60:MET:CE	1:A:66:PRO:CB	2.71	0.66
1:A:39:VAL:HG12	1:A:41:GLY:O	1.96	0.66
1:C:68:ARG:HH22	2:D:115:SER:HB2	1.61	0.66
1:A:59:ILE:CG2	2:B:124:PHE:CE2	2.78	0.66
2:H:76:ARG:HB3	2:H:143:ILE:HG12	1.78	0.65
1:E:400:ILE:HD13	1:E:411:PHE:CE2	2.31	0.65
1:G:299:SER:HA	1:G:307:CYS:HA	1.78	0.65
1:C:118:CYS:N	1:G:115:MET:SD	2.69	0.65
1:A:386:TYR:CD1	1:A:390:GLN:HG3	2.31	0.65
1:G:69:THR:CG2	1:G:70:TYR:N	2.59	0.65
1:E:342:THR:HG23	1:E:403:LEU:O	1.95	0.65
1:G:73:CYS:HB2	2:H:123:PRO:HG3	1.78	0.65
1:E:155:THR:CG2	1:E:156:GLN:H	2.10	0.65
1:G:164:MET:O	1:G:165:LYS:HB2	1.96	0.65
1:E:155:THR:CG2	1:E:156:GLN:N	2.60	0.65
1:C:317:ASP:HB2	1:C:421:LYS:NZ	2.12	0.65
1:G:37:ARG:HD3	1:G:67:ILE:HD13	1.80	0.64
1:G:338:ASN:CB	1:G:345:ASN:HB2	2.25	0.64
1:C:473:GLU:OE1	1:C:516:ARG:NH1	2.30	0.64
1:A:406:HIS:CG	1:A:469:GLY:HA2	2.31	0.64
2:B:74:THR:O	2:B:76:ARG:NH1	2.31	0.64
1:E:385:HIS:CA	1:E:386:TYR:HB2	2.17	0.64
1:E:67:ILE:CG2	1:E:68:ARG:N	2.60	0.64
1:A:114:VAL:C	1:E:115:MET:HB2	2.18	0.64
1:A:372:GLY:C	1:A:374:PRO:HD2	2.17	0.64
1:G:294:PRO:HG2	1:G:322:SER:O	1.90	0.64
1:G:298:TYR:C	1:G:307:CYS:CB	2.65	0.64
1:A:354:THR:HG23	1:A:356:GLY:HA3	1.79	0.64
2:H:55:ASN:N	2:H:118:PHE:O	2.25	0.64
1:C:115:MET:CG	1:G:115:MET:O	2.46	0.63
1:C:317:ASP:HB2	1:C:421:LYS:HZ3	1.62	0.63
1:G:69:THR:HG22	1:G:70:TYR:N	2.12	0.63
1:G:164:MET:O	1:G:165:LYS:CB	2.47	0.63
1:A:438:GLN:NE2	1:A:518:ALA:HB3	2.13	0.63
1:A:117:THR:OG1	1:E:115:MET:CE	2.46	0.63
1:G:162:ARG:NH1	2:H:126:LEU:HB3	2.14	0.63
2:F:32:TYR:CD2	2:F:52:VAL:HG12	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HD12	1:C:35:ASP:N	2.14	0.63
1:G:335:LEU:CD1	1:G:346:LEU:CD2	2.73	0.63
1:C:43:LEU:HD11	1:C:45:TRP:HE1	1.63	0.62
2:H:119:GLN:HE21	2:H:122:THR:HG22	1.64	0.62
1:C:354:THR:C	1:C:356:GLY:HA2	2.20	0.62
1:C:115:MET:HA	1:G:115:MET:O	1.99	0.62
2:H:104:ARG:NH1	2:H:108:PRO:HD3	2.14	0.62
1:A:59:ILE:HG21	2:B:124:PHE:CE2	2.34	0.62
1:C:58:SER:C	1:C:59:ILE:HG13	2.20	0.62
1:G:67:ILE:HG22	1:G:68:ARG:N	2.14	0.62
1:C:294:PRO:HB3	1:C:322:SER:O	2.00	0.62
2:B:36:TRP:HB3	2:B:77:TYR:OH	2.01	0.61
1:G:69:THR:HG23	1:G:194:LEU:O	2.01	0.61
2:H:124:PHE:CE2	2:H:126:LEU:HB2	2.34	0.61
1:C:68:ARG:NH2	2:D:115:SER:HB2	2.15	0.61
2:F:103:ASN:HB3	2:F:143:ILE:HD12	1.82	0.61
1:E:401:THR:HG22	1:E:402:ASP:N	2.15	0.61
2:B:76:ARG:NH2	2:B:144:PRO:HD3	2.15	0.61
1:C:39:VAL:HB	1:C:43:LEU:HD22	1.82	0.61
1:C:295:PRO:O	1:C:325:CYS:N	2.33	0.61
1:A:43:LEU:HD12	1:A:43:LEU:O	2.01	0.61
2:H:121:PHE:HA	2:H:129:GLU:OE2	2.01	0.61
1:A:335:LEU:HD12	1:A:346:LEU:HD21	1.81	0.61
1:C:118:CYS:H	1:G:115:MET:HE1	1.64	0.60
1:C:65:THR:O	1:C:67:ILE:HG22	2.00	0.60
2:F:32:TYR:HD2	2:F:52:VAL:HG12	1.66	0.60
1:E:371:ALA:HB2	4:E:3402:NAG:H61	1.81	0.60
2:H:78:VAL:HG12	2:H:80:TYR:CE1	2.36	0.60
1:A:69:THR:HB	1:A:194:LEU:O	2.01	0.60
1:C:60:MET:HE1	1:C:66:PRO:HB3	1.83	0.60
1:A:335:LEU:HD22	1:A:430:VAL:HG13	1.82	0.60
1:E:175:PRO:HB3	1:E:221:ALA:HB1	1.84	0.60
2:B:95:LYS:HE2	2:B:95:LYS:HA	1.83	0.60
1:C:66:PRO:C	1:C:67:ILE:HG22	2.21	0.60
1:E:307:CYS:HB2	1:E:315:ARG:HH22	1.66	0.60
1:C:39:VAL:HG21	1:C:43:LEU:HD13	1.83	0.60
1:A:61:ASP:OD2	1:A:67:ILE:HD13	2.01	0.60
1:A:403:LEU:HB2	1:A:409:TYR:OH	2.01	0.60
1:C:314:PHE:HB2	1:C:419:VAL:HG11	1.84	0.60
1:C:237:SER:HB2	1:C:261:LEU:O	2.01	0.60
1:C:39:VAL:HG11	1:C:43:LEU:CB	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:PRO:HG3	1:E:413:ILE:HG22	1.84	0.59
1:G:406:HIS:ND1	1:G:469:GLY:HA2	2.17	0.59
1:C:155:THR:HG22	1:C:156:GLN:H	1.64	0.59
2:D:65:TYR:CD2	2:D:74:THR:HG22	2.36	0.59
1:C:389:GLN:HB2	1:C:393:LEU:HD13	1.85	0.59
1:G:328:PRO:HB3	1:G:420:SER:HB3	1.84	0.59
1:A:340:ASN:OD1	1:A:341:GLU:N	2.35	0.59
1:C:114:VAL:O	1:G:115:MET:CE	2.51	0.59
2:D:129:GLU:HB3	2:D:131:ARG:HH12	1.67	0.59
1:G:270:SER:OG	1:G:271:GLY:N	2.35	0.59
1:C:226:LEU:HD21	1:C:254:LEU:HD12	1.84	0.59
2:F:73:LYS:NZ	2:F:73:LYS:HA	2.17	0.59
1:A:386:TYR:H	1:A:400:ILE:HA	1.67	0.59
1:G:162:ARG:NH2	2:H:128:PHE:CZ	2.71	0.59
1:C:328:PRO:HB3	1:C:420:SER:HB3	1.84	0.58
1:E:382:SER:OG	1:E:384:VAL:HG13	2.03	0.58
1:C:69:THR:HB	1:C:194:LEU:O	2.03	0.58
1:A:406:HIS:CE1	1:A:469:GLY:HA3	2.39	0.58
1:G:386:TYR:CE1	1:G:390:GLN:HG3	2.38	0.58
1:G:390:GLN:O	1:G:391:ASN:ND2	2.36	0.58
1:C:61:ASP:CG	1:C:67:ILE:HG21	2.23	0.58
2:H:117:LYS:HG2	2:H:119:GLN:HB3	1.86	0.58
1:G:61:ASP:O	1:G:63:LYS:N	2.37	0.58
1:C:342:THR:HB	1:C:403:LEU:O	2.04	0.58
1:E:63:LYS:O	1:E:64:ASN:HB2	2.03	0.58
1:A:357:ARG:NH1	1:A:418:GLY:H	2.02	0.58
1:A:109:ASN:OD1	1:E:116:GLY:O	2.22	0.58
1:E:357:ARG:HG3	1:E:359:ASP:OD1	2.04	0.58
1:G:373:ASP:N	1:G:374:PRO:HD2	2.19	0.58
1:A:384:VAL:HG12	1:A:402:ASP:O	2.04	0.58
1:C:294:PRO:HG2	1:C:315:ARG:NH1	2.17	0.57
1:C:115:MET:HG3	1:G:115:MET:O	2.04	0.57
2:D:64:HIS:H	4:D:201:NAG:H81	1.70	0.57
1:C:155:THR:CG2	1:C:156:GLN:H	2.17	0.57
1:G:245:MET:SD	1:G:256:PRO:HB3	2.44	0.57
1:G:112:PRO:O	1:G:114:VAL:HG13	2.04	0.57
1:G:340:ASN:CG	1:G:341:GLU:H	2.07	0.57
1:C:105:LEU:HD21	1:C:120:GLU:HG3	1.85	0.57
1:C:118:CYS:CB	1:G:115:MET:HE1	2.17	0.57
1:G:405:ALA:O	1:G:436:THR:CB	2.46	0.57
2:F:152:LEU:H	2:F:152:LEU:HD12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HB3	1:A:221:ALA:HB1	1.87	0.57
1:G:299:SER:CA	1:G:307:CYS:HA	2.35	0.57
1:A:115:MET:O	1:E:115:MET:SD	2.63	0.57
2:D:32:TYR:CD2	2:D:32:TYR:N	2.71	0.57
1:G:386:TYR:CD1	1:G:390:GLN:HG3	2.39	0.57
1:C:314:PHE:N	1:C:326:THR:O	2.38	0.57
1:E:316:ALA:O	1:E:319:ASP:HB2	2.05	0.57
1:A:155:THR:CG2	1:A:156:GLN:N	2.68	0.57
1:C:403:LEU:HD13	1:C:409:TYR:CE1	2.40	0.57
2:F:65:TYR:CD2	2:F:74:THR:HG22	2.40	0.57
1:C:155:THR:HG22	1:C:157:VAL:H	1.70	0.56
1:G:193:ALA:HB2	2:H:123:PRO:HB2	1.87	0.56
1:E:328:PRO:HB3	1:E:420:SER:CB	2.35	0.56
1:E:270:SER:OG	1:E:271:GLY:N	2.36	0.56
1:G:406:HIS:CG	1:G:469:GLY:HA2	2.40	0.56
2:H:99:ARG:NE	2:H:128:PHE:CE2	2.73	0.56
1:E:317:ASP:OD1	1:E:422:TYR:OH	2.24	0.56
2:B:36:TRP:O	2:B:152:LEU:HD13	2.05	0.56
1:G:192:ILE:HG12	1:G:193:ALA:N	2.19	0.56
1:A:341:GLU:C	1:A:437:ASN:HB3	2.24	0.56
1:A:414:TRP:CH2	1:A:426:PRO:HA	2.41	0.56
1:C:139:GLU:C	1:C:142:PHE:CE2	2.79	0.56
1:C:61:ASP:OD1	1:C:67:ILE:HG21	2.05	0.56
1:C:68:ARG:HH22	2:D:115:SER:CB	2.19	0.56
2:F:162:ASN:OD1	2:F:162:ASN:N	2.37	0.56
1:C:386:TYR:HB3	1:C:390:GLN:HB2	1.86	0.56
1:E:40:GLN:C	1:E:41:GLY:O	2.44	0.56
2:H:77:TYR:H	2:H:102:CYS:HB2	1.71	0.56
1:C:328:PRO:HB3	1:C:420:SER:HB2	1.88	0.56
1:G:155:THR:CG2	1:G:156:GLN:N	2.69	0.55
1:A:116:GLY:N	1:E:115:MET:CB	2.68	0.55
1:A:115:MET:N	1:E:115:MET:HB2	2.20	0.55
2:H:87:TYR:HE1	2:H:153:LYS:HB3	1.68	0.55
2:D:74:THR:OG1	2:D:76:ARG:NH1	2.38	0.55
1:E:59:ILE:CG2	1:E:60:MET:H	2.17	0.55
1:C:60:MET:CE	1:C:66:PRO:HB3	2.35	0.55
1:C:244:LYS:HB2	1:C:257:ILE:HG13	1.88	0.55
1:E:385:HIS:O	1:E:401:THR:HB	2.07	0.55
1:E:69:THR:HB	1:E:194:LEU:O	2.06	0.55
1:G:59:ILE:CG2	1:G:60:MET:N	2.68	0.55
2:F:103:ASN:HB3	2:F:143:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:SER:HB2	1:G:138:ARG:NH2	2.20	0.55
1:C:294:PRO:CG	1:C:315:ARG:HH11	2.19	0.55
2:F:104:ARG:HB2	2:F:112:LEU:HD22	1.88	0.55
1:C:373:ASP:C	1:C:375:SER:H	2.10	0.55
2:F:28:VAL:CG1	2:F:29:ALA:N	2.70	0.55
1:G:382:SER:OG	1:G:384:VAL:HG13	2.07	0.55
1:A:328:PRO:HB3	1:A:420:SER:CB	2.36	0.55
1:A:406:HIS:CD2	1:A:469:GLY:HA2	2.41	0.55
1:C:382:SER:OG	1:C:383:GLY:N	2.39	0.55
1:C:355:GLY:N	1:C:356:GLY:HA2	2.22	0.55
1:E:355:GLY:N	1:E:356:GLY:HA2	2.22	0.55
1:E:37:ARG:CD	1:E:67:ILE:HD11	2.37	0.55
1:C:421:LYS:HE3	1:C:422:TYR:CZ	2.42	0.55
1:G:124:LEU:HG	1:G:145:ILE:HD12	1.89	0.55
1:G:37:ARG:HD3	1:G:67:ILE:CD1	2.36	0.54
1:A:512:HIS:HE1	1:A:527:PRO:HG3	1.72	0.54
2:F:65:TYR:CE2	2:F:74:THR:HB	2.42	0.54
1:E:342:THR:O	1:E:342:THR:CG2	2.55	0.54
1:C:105:LEU:CD2	1:C:120:GLU:HG3	2.37	0.54
1:A:161:ASP:O	1:A:162:ARG:CB	2.54	0.54
2:B:64:HIS:O	4:B:201:NAG:H83	2.08	0.54
1:G:385:HIS:HA	1:G:386:TYR:CB	2.15	0.54
1:A:406:HIS:NE2	1:A:469:GLY:HA2	2.22	0.54
1:C:295:PRO:HG2	1:C:324:PRO:CB	2.25	0.54
1:A:114:VAL:C	1:E:115:MET:CE	2.76	0.54
1:E:379:PRO:O	1:E:380:CYS:SG	2.66	0.54
1:G:406:HIS:O	4:G:3402:NAG:H81	2.08	0.54
1:E:335:LEU:HD13	1:E:346:LEU:HD21	1.89	0.54
1:C:296:HIS:HB2	1:C:325:CYS:HB2	1.90	0.54
2:B:57:TYR:CE1	2:B:117:LYS:HB2	2.43	0.54
2:H:82:VAL:HG12	2:H:95:LYS:O	2.08	0.54
2:F:164:CYS:O	2:F:165:MET:CG	2.56	0.54
1:E:386:TYR:CD1	1:E:390:GLN:HG3	2.43	0.53
1:C:390:GLN:HG2	1:C:390:GLN:O	2.08	0.53
2:D:126:LEU:HD23	2:D:126:LEU:N	2.22	0.53
2:B:31:ARG:NH1	2:B:59:ASP:OD2	2.40	0.53
1:E:106:ARG:HB3	1:E:191:CYS:HB3	1.90	0.53
1:A:448:GLN:HG2	1:A:460:ALA:O	2.09	0.53
1:E:129:SER:HB2	1:E:138:ARG:NH2	2.22	0.53
1:E:112:PRO:O	1:E:114:VAL:HG13	2.08	0.53
1:G:63:LYS:O	1:G:64:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:PRO:HB3	1:E:420:SER:HB3	1.89	0.53
1:A:437:ASN:OD1	1:A:438:GLN:N	2.40	0.53
2:F:52:VAL:O	2:F:159:ARG:HG2	2.08	0.53
1:G:328:PRO:HB3	1:G:420:SER:CB	2.38	0.53
1:C:73:CYS:HB2	2:D:123:PRO:CG	2.23	0.53
1:G:386:TYR:H	1:G:400:ILE:HA	1.74	0.53
1:G:164:MET:O	1:G:165:LYS:HG3	2.08	0.53
1:G:175:PRO:HB3	1:G:221:ALA:HB1	1.89	0.53
1:C:379:PRO:O	1:C:380:CYS:CB	2.56	0.53
1:A:126:TYR:CE1	1:A:143:VAL:HG22	2.44	0.53
2:H:99:ARG:NH2	2:H:116:GLU:OE1	2.42	0.53
1:C:486:ARG:HD3	1:C:488:TYR:CZ	2.45	0.52
2:H:40:ASN:O	2:H:44:GLN:HG3	2.09	0.52
1:E:414:TRP:CH2	1:E:426:PRO:HA	2.44	0.52
1:A:138:ARG:HD3	1:A:141:GLN:HB2	1.90	0.52
1:A:114:VAL:O	1:E:115:MET:SD	2.67	0.52
2:D:65:TYR:CE2	2:D:74:THR:HA	2.45	0.52
1:G:414:TRP:CH2	1:G:426:PRO:HA	2.44	0.52
1:C:37:ARG:HG2	1:C:67:ILE:HD12	1.92	0.52
2:F:43:PHE:CD1	2:F:152:LEU:HB3	2.44	0.52
1:C:357:ARG:HH11	1:C:357:ARG:HG3	1.73	0.52
1:A:228:GLU:HB2	1:A:246:TYR:CE1	2.44	0.52
2:D:100:TRP:CG	2:D:114:PHE:HB2	2.44	0.52
2:F:148:ARG:HD2	2:F:150:SER:OG	2.10	0.52
2:D:159:ARG:HD2	2:D:163:SER:HB2	1.91	0.52
2:H:65:TYR:HE2	2:H:74:THR:HG1	1.58	0.52
2:H:74:THR:HG23	2:H:76:ARG:HH11	1.74	0.52
1:G:357:ARG:HH12	1:G:418:GLY:CA	2.23	0.52
1:G:155:THR:CG2	1:G:156:GLN:H	2.17	0.52
1:A:59:ILE:HG22	1:A:60:MET:N	2.25	0.51
1:E:326:THR:HG21	1:E:357:ARG:HE	1.75	0.51
1:G:45:TRP:HB3	1:G:85:ARG:O	2.10	0.51
2:F:98:LYS:HZ1	2:F:101:GLU:CD	2.13	0.51
1:G:57:VAL:HG22	1:G:58:SER:H	1.74	0.51
1:G:406:HIS:HB2	1:G:469:GLY:N	2.24	0.51
2:B:99:ARG:NH1	2:B:114:PHE:CZ	2.79	0.51
2:B:126:LEU:HD23	2:B:126:LEU:N	2.26	0.51
1:C:39:VAL:HG12	1:C:43:LEU:HB2	1.90	0.51
1:C:296:HIS:HA	1:C:310:ASP:OD2	2.11	0.51
1:C:43:LEU:HD11	1:C:45:TRP:NE1	2.26	0.51
2:F:145:ASP:OD1	2:F:146:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:HG2	1:G:115:MET:O	2.10	0.51
1:C:124:LEU:HG	1:C:145:ILE:HD12	1.92	0.51
2:H:31:ARG:NH1	2:H:59:ASP:OD2	2.44	0.51
2:D:87:TYR:CE1	2:D:153:LYS:HD3	2.45	0.51
1:E:369:CYS:O	1:E:408:ASN:HB2	2.10	0.51
1:E:226:LEU:HD21	1:E:254:LEU:HD12	1.93	0.51
1:A:406:HIS:ND1	1:A:469:GLY:CA	2.73	0.51
1:G:406:HIS:CG	1:G:406:HIS:O	2.63	0.51
1:G:35:ASP:O	1:G:39:VAL:HB	2.11	0.51
1:A:59:ILE:HG23	2:B:124:PHE:CE2	2.46	0.51
1:A:34:LEU:HD12	1:A:35:ASP:N	2.26	0.51
1:C:109:ASN:OD1	1:G:116:GLY:O	2.28	0.51
1:G:406:HIS:HB2	1:G:468:ASN:C	2.32	0.50
1:A:61:ASP:OD2	1:A:67:ILE:HG21	2.11	0.50
1:G:357:ARG:HG3	1:G:359:ASP:OD1	2.11	0.50
1:G:342:THR:HG23	1:G:401:THR:HG22	1.93	0.50
1:E:390:GLN:O	1:E:391:ASN:ND2	2.44	0.50
1:G:344:VAL:HG11	1:G:400:ILE:HD13	1.93	0.50
1:C:57:VAL:CG1	1:C:59:ILE:HD12	2.29	0.50
1:G:59:ILE:HG23	2:H:124:PHE:CE2	2.47	0.50
1:A:114:VAL:O	1:E:115:MET:CE	2.59	0.50
1:E:309:CYS:SG	1:E:315:ARG:HB2	2.52	0.50
1:A:407:THR:O	1:A:436:THR:OG1	2.29	0.50
1:A:354:THR:C	1:A:356:GLY:HA2	2.32	0.50
1:E:27:PRO:HB2	1:E:29:ASN:OD1	2.11	0.50
2:H:63:PRO:HA	4:H:201:NAG:O7	2.12	0.50
2:F:36:TRP:HZ2	2:F:140:SER:HG	1.59	0.50
1:E:318:ASN:N	1:E:318:ASN:OD1	2.44	0.50
1:A:385:HIS:HA	1:A:386:TYR:CB	2.28	0.50
2:B:159:ARG:HD3	2:B:163:SER:HB2	1.94	0.50
1:G:344:VAL:HG12	1:G:345:ASN:N	2.26	0.50
2:F:28:VAL:HG12	2:F:29:ALA:H	1.77	0.50
1:A:61:ASP:CG	1:A:67:ILE:HD13	2.32	0.50
1:C:357:ARG:NH1	1:C:418:GLY:H	2.09	0.50
1:A:346:LEU:HD23	1:A:347:GLU:N	2.27	0.50
1:E:46:ILE:HD13	1:E:46:ILE:H	1.75	0.50
1:C:56:GLU:HA	1:C:69:THR:O	2.12	0.50
2:F:85:ASP:OD1	2:F:85:ASP:N	2.44	0.50
1:C:368:LYS:O	1:C:377:CYS:HA	2.12	0.50
1:C:85:ARG:HD3	1:C:137:ILE:HG12	1.94	0.50
2:H:54:ILE:HG13	2:H:158:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:O	1:A:162:ARG:HB3	2.12	0.49
1:E:339:VAL:O	1:E:339:VAL:HG23	2.12	0.49
1:A:342:THR:HG21	1:A:403:LEU:O	2.07	0.49
1:G:105:LEU:HD21	1:G:120:GLU:HG3	1.94	0.49
1:A:328:PRO:HB3	1:A:420:SER:HB3	1.94	0.49
1:A:374:PRO:O	1:A:375:SER:HB2	2.13	0.49
1:E:59:ILE:O	1:E:66:PRO:HA	2.12	0.49
2:H:119:GLN:HE21	2:H:122:THR:CG2	2.25	0.49
1:A:59:ILE:CG2	1:A:60:MET:N	2.75	0.49
1:A:118:CYS:N	1:E:115:MET:HG2	2.10	0.49
1:A:357:ARG:HG3	1:A:359:ASP:OD1	2.12	0.49
1:C:126:TYR:CE1	1:C:143:VAL:HG22	2.48	0.49
1:A:473:GLU:HG2	1:A:516:ARG:HH11	1.77	0.49
1:A:118:CYS:H	1:E:115:MET:CG	2.13	0.49
2:H:65:TYR:HB2	2:H:69:VAL:HG21	1.94	0.49
1:E:63:LYS:O	1:E:64:ASN:CB	2.59	0.49
1:G:367:LYS:HB3	1:G:377:CYS:HB2	1.94	0.49
1:C:114:VAL:HG23	1:G:115:MET:HE2	1.95	0.49
1:G:405:ALA:HB3	1:G:468:ASN:HB3	1.95	0.49
1:E:37:ARG:HD3	1:E:67:ILE:HD11	1.95	0.49
1:E:51:GLU:OE2	2:F:28:VAL:HG13	2.13	0.49
1:G:298:TYR:N	1:G:307:CYS:HB3	2.28	0.49
1:G:102:LYS:HD3	1:G:166:LEU:HD21	1.95	0.49
1:A:346:LEU:HD23	1:A:347:GLU:H	1.78	0.49
2:B:99:ARG:HH22	2:B:116:GLU:CD	2.17	0.49
1:C:138:ARG:HD3	1:C:141:GLN:HB2	1.93	0.49
1:E:102:LYS:HA	1:E:167:ASN:O	2.13	0.49
4:E:3403:NAG:H3	4:E:3403:NAG:H83	1.94	0.49
1:A:61:ASP:OD1	1:A:67:ILE:HD13	2.13	0.48
1:A:164:MET:HB2	2:B:126:LEU:HG	1.95	0.48
1:G:320:ALA:HB3	1:G:323:MET:HG3	1.93	0.48
1:E:313:PHE:HB3	1:E:325:CYS:HB3	1.95	0.48
1:G:157:VAL:O	1:G:157:VAL:HG12	2.14	0.48
1:A:116:GLY:H	1:E:115:MET:CB	2.26	0.48
1:E:59:ILE:HG23	1:E:60:MET:H	1.78	0.48
1:C:439:ALA:C	1:C:519:ALA:HB3	2.33	0.48
2:F:28:VAL:CG1	2:F:29:ALA:H	2.25	0.48
2:F:67:ASP:HA	2:F:106:HIS:ND1	2.29	0.48
1:E:228:GLU:HB2	1:E:246:TYR:CE1	2.49	0.48
1:C:366:CYS:SG	1:C:367:LYS:N	2.86	0.48
1:A:58:SER:O	1:A:59:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:GLN:O	1:E:41:GLY:O	2.31	0.48
1:A:211:LEU:HD21	1:A:268:GLU:HG3	1.95	0.48
1:G:355:GLY:N	1:G:356:GLY:HA2	2.28	0.48
1:G:436:THR:HG22	1:G:437:ASN:N	2.28	0.48
1:C:39:VAL:CB	1:C:43:LEU:HB2	2.43	0.48
1:G:61:ASP:O	1:G:64:ASN:N	2.46	0.48
1:G:106:ARG:HB3	1:G:191:CYS:HB3	1.94	0.48
1:C:294:PRO:HG3	1:C:321:ALA:O	2.13	0.48
2:H:60:VAL:HG11	2:H:79:LEU:HD11	1.96	0.48
1:G:294:PRO:HD3	1:G:322:SER:HA	1.96	0.48
1:A:362:TYR:HA	1:A:414:TRP:O	2.13	0.48
1:C:373:ASP:O	1:C:375:SER:N	2.43	0.47
1:C:386:TYR:H	1:C:400:ILE:HA	1.79	0.47
2:F:119:GLN:HE22	2:F:122:THR:HG23	1.79	0.47
2:B:99:ARG:NH1	2:B:114:PHE:HZ	2.12	0.47
2:F:38:SER:C	2:F:40:ASN:H	2.18	0.47
2:F:100:TRP:CZ2	2:F:113:LYS:O	2.67	0.47
1:G:211:LEU:HD21	1:G:268:GLU:HG3	1.94	0.47
1:G:105:LEU:HD21	1:G:120:GLU:CG	2.45	0.47
1:C:118:CYS:CA	1:G:115:MET:HE3	2.42	0.47
1:G:338:ASN:HB3	1:G:345:ASN:CB	2.33	0.47
1:G:338:ASN:HB3	1:G:345:ASN:HD22	1.79	0.47
2:F:119:GLN:NE2	2:F:122:THR:HG23	2.29	0.47
1:C:239:GLU:HG3	1:C:239:GLU:O	2.13	0.47
1:E:406:HIS:CG	1:E:469:GLY:HA2	2.49	0.47
1:C:115:MET:HE2	1:G:114:VAL:CA	2.20	0.47
2:H:38:SER:C	2:H:40:ASN:H	2.17	0.47
1:E:357:ARG:HH12	1:E:418:GLY:CA	2.26	0.47
2:B:81:MET:O	2:B:96:GLY:HA3	2.14	0.47
1:G:102:LYS:HA	1:G:167:ASN:O	2.15	0.47
1:G:67:ILE:CG2	1:G:68:ARG:N	2.77	0.47
1:G:342:THR:HG23	1:G:401:THR:CG2	2.45	0.47
1:G:439:ALA:C	1:G:519:ALA:HB3	2.35	0.47
2:H:36:TRP:CE3	2:H:43:PHE:HZ	2.31	0.47
1:G:298:TYR:O	1:G:307:CYS:C	2.53	0.47
1:C:403:LEU:HD13	1:C:409:TYR:CZ	2.50	0.47
1:E:319:ASP:OD1	1:E:320:ALA:N	2.48	0.47
1:A:226:LEU:HD11	1:E:254:LEU:HD13	1.95	0.47
1:C:43:LEU:HG	1:C:43:LEU:O	2.14	0.47
2:H:85:ASP:HB3	2:H:95:LYS:HE2	1.97	0.47
2:B:54:ILE:HD12	2:B:158:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:TYR:H	2:D:102:CYS:HB2	1.80	0.47
2:H:58:LEU:HB3	2:H:116:GLU:HB3	1.96	0.47
2:F:65:TYR:CD2	2:F:74:THR:HB	2.50	0.46
1:A:226:LEU:CD1	1:E:254:LEU:HD13	2.45	0.46
1:C:362:TYR:HA	1:C:414:TRP:O	2.14	0.46
1:A:316:ALA:O	1:A:319:ASP:HB2	2.15	0.46
2:F:87:TYR:HE1	2:F:153:LYS:HB2	1.80	0.46
1:A:386:TYR:CE1	1:A:390:GLN:HG3	2.50	0.46
1:C:61:ASP:OD1	1:C:67:ILE:HD13	2.16	0.46
1:C:420:SER:C	1:C:422:TYR:N	2.67	0.46
2:D:76:ARG:HB2	2:D:143:ILE:HB	1.97	0.46
1:A:98:TYR:CD2	1:A:172:ASP:HB3	2.51	0.46
1:C:406:HIS:O	1:C:406:HIS:CG	2.67	0.46
1:E:341:GLU:O	1:E:436:THR:HG22	2.14	0.46
1:A:341:GLU:HA	1:A:437:ASN:ND2	2.31	0.46
1:E:138:ARG:O	1:E:142:PHE:CE2	2.68	0.46
1:G:57:VAL:HG22	1:G:58:SER:N	2.30	0.46
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.74	0.46
1:A:315:ARG:HD3	1:A:319:ASP:OD1	2.15	0.46
2:B:122:THR:HG22	2:B:124:PHE:N	2.16	0.46
1:C:379:PRO:O	1:C:380:CYS:SG	2.73	0.46
1:G:357:ARG:HH12	1:G:418:GLY:HA3	1.79	0.46
1:A:226:LEU:HD21	1:A:254:LEU:HD12	1.98	0.46
1:A:155:THR:CG2	1:A:156:GLN:H	2.29	0.46
2:D:74:THR:O	2:D:76:ARG:NH1	2.49	0.46
2:D:121:PHE:HA	2:D:129:GLU:OE2	2.16	0.46
1:E:406:HIS:O	1:E:406:HIS:CG	2.67	0.46
2:F:133:GLY:O	2:F:134:ARG:HG3	2.14	0.46
1:A:115:MET:HA	1:E:115:MET:CA	2.44	0.46
1:A:385:HIS:CA	1:A:386:TYR:HB2	2.31	0.46
1:C:440:ALA:N	1:C:519:ALA:HB3	2.31	0.46
2:F:65:TYR:CD2	2:F:74:THR:CG2	2.99	0.46
1:G:472:LEU:HG	1:G:517:THR:HA	1.98	0.46
1:G:297:SER:HB2	1:G:315:ARG:NH1	2.31	0.46
1:C:226:LEU:CD2	1:C:254:LEU:HD12	2.46	0.46
1:C:314:PHE:HB2	1:C:419:VAL:CG1	2.46	0.46
2:F:74:THR:OG1	2:F:76:ARG:NH1	2.49	0.46
2:H:43:PHE:CD1	2:H:152:LEU:HD12	2.51	0.46
1:C:254:LEU:HD13	1:G:226:LEU:HD11	1.94	0.45
1:C:386:TYR:CD1	1:C:390:GLN:HG3	2.51	0.45
1:A:155:THR:HG22	1:A:156:GLN:H	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ARG:NE	2:B:128:PHE:CE2	2.84	0.45
1:A:439:ALA:HA	1:A:519:ALA:HB1	1.98	0.45
1:A:355:GLY:N	1:A:356:GLY:HA2	2.31	0.45
1:E:138:ARG:HD3	1:E:141:GLN:HB2	1.98	0.45
1:E:138:ARG:O	1:E:142:PHE:CD2	2.69	0.45
1:G:58:SER:HB2	2:H:100:TRP:CZ3	2.51	0.45
2:H:74:THR:HG23	2:H:76:ARG:HD3	1.98	0.45
1:E:67:ILE:HG21	1:E:67:ILE:HD13	1.68	0.45
1:C:34:LEU:HD12	1:C:35:ASP:H	1.79	0.45
2:H:147:GLY:C	2:H:149:ARG:H	2.19	0.45
2:H:131:ARG:O	2:H:134:ARG:HB2	2.16	0.45
1:A:58:SER:C	1:A:59:ILE:HG13	2.37	0.45
2:B:119:GLN:NE2	2:B:122:THR:HA	2.32	0.45
1:A:116:GLY:H	1:E:115:MET:CA	2.28	0.45
1:A:403:LEU:HB2	1:A:409:TYR:CZ	2.52	0.45
1:C:254:LEU:HD23	1:C:254:LEU:HA	1.85	0.45
1:A:126:TYR:CE1	1:A:143:VAL:CG2	3.00	0.45
1:G:368:LYS:N	1:G:377:CYS:HB3	2.32	0.45
1:A:364:VAL:HG21	1:A:398:VAL:HG11	1.97	0.45
1:A:88:TRP:CE2	1:A:180:GLY:HA3	2.52	0.45
1:E:48:SER:HB3	1:E:137:ILE:HD12	1.99	0.45
1:G:344:VAL:CG1	1:G:345:ASN:N	2.78	0.45
1:A:114:VAL:O	1:E:115:MET:HE3	2.16	0.45
2:B:74:THR:HG21	2:B:105:PRO:HG2	1.96	0.45
2:B:85:ASP:HB2	2:B:95:LYS:HZ2	1.81	0.45
1:E:357:ARG:HH12	1:E:418:GLY:HA3	1.82	0.45
1:G:412:GLU:HG2	1:G:431:SER:OG	2.16	0.45
1:C:61:ASP:OD2	1:C:67:ILE:HG21	2.17	0.45
1:C:139:GLU:C	1:C:142:PHE:HE2	2.18	0.45
1:A:114:VAL:C	1:E:115:MET:CB	2.74	0.45
2:B:148:ARG:CB	2:B:150:SER:O	2.60	0.45
1:G:59:ILE:O	1:G:66:PRO:HA	2.17	0.45
1:E:320:ALA:C	1:E:322:SER:H	2.18	0.45
2:D:99:ARG:NH2	2:D:116:GLU:OE1	2.50	0.45
1:E:139:GLU:HG2	1:E:139:GLU:H	1.51	0.45
1:A:139:GLU:C	1:A:142:PHE:CE2	2.90	0.45
1:G:240:LYS:HD2	1:G:261:LEU:HD11	1.99	0.45
1:C:59:ILE:HG23	2:D:124:PHE:CE2	2.52	0.45
2:F:117:LYS:HG2	2:F:119:GLN:HB3	1.99	0.44
1:C:129:SER:HB2	1:C:138:ARG:NH2	2.32	0.44
1:E:265:GLY:O	1:E:303:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:146:ASN:HB2	2:F:148:ARG:HG2	1.98	0.44
1:G:487:SER:OG	1:G:489:ARG:HD2	2.16	0.44
1:G:226:LEU:CD2	1:G:254:LEU:HD12	2.45	0.44
2:F:89:ALA:HB1	2:F:149:ARG:HH12	1.82	0.44
2:F:135:GLU:HA	2:F:156:VAL:O	2.18	0.44
1:E:401:THR:CG2	1:E:402:ASP:N	2.81	0.44
1:G:373:ASP:HB2	1:G:374:PRO:HD3	1.99	0.44
1:E:75:VAL:HG21	1:E:111:LEU:HD13	1.98	0.44
1:E:335:LEU:HD11	1:E:346:LEU:HD21	1.95	0.44
1:E:316:ALA:C	1:E:319:ASP:HB2	2.37	0.44
1:E:320:ALA:C	1:E:322:SER:N	2.70	0.44
2:H:76:ARG:NH2	2:H:143:ILE:CG2	2.79	0.44
2:D:76:ARG:HE	2:D:143:ILE:HG21	1.83	0.44
1:G:362:TYR:HA	1:G:414:TRP:O	2.18	0.44
1:G:366:CYS:SG	1:G:367:LYS:N	2.90	0.44
1:G:126:TYR:CE1	1:G:143:VAL:HG22	2.53	0.44
1:C:364:VAL:HG21	1:C:398:VAL:HG11	2.00	0.44
1:G:506:LEU:HA	1:G:532:THR:O	2.17	0.44
1:G:233:CYS:SG	1:G:239:GLU:HB3	2.58	0.44
2:F:164:CYS:O	2:F:165:MET:HG2	2.16	0.44
1:E:126:TYR:CE1	1:E:143:VAL:HG22	2.53	0.44
1:G:340:ASN:OD1	1:G:341:GLU:N	2.51	0.43
1:G:129:SER:HB2	1:G:138:ARG:HH22	1.83	0.43
1:E:414:TRP:CD2	1:E:429:SER:HB3	2.53	0.43
2:D:159:ARG:HD2	2:D:163:SER:CB	2.48	0.43
1:A:443:SER:HB3	1:A:523:ASP:HB2	2.00	0.43
1:A:94:ALA:HB2	1:A:201:TYR:CG	2.52	0.43
1:G:339:VAL:HG22	1:G:343:SER:O	2.18	0.43
2:B:74:THR:O	2:B:74:THR:HG22	2.18	0.43
1:E:351:PRO:HD3	1:E:362:TYR:OH	2.18	0.43
1:A:373:ASP:H	1:A:374:PRO:HD2	1.72	0.43
1:E:67:ILE:HG22	1:E:68:ARG:O	2.18	0.43
2:B:54:ILE:CD1	2:B:158:VAL:HG11	2.48	0.43
1:A:245:MET:SD	1:A:256:PRO:HB3	2.59	0.43
2:F:31:ARG:NH1	2:F:59:ASP:OD1	2.51	0.43
1:A:537:SER:HB3	1:A:540:ILE:HD12	2.00	0.43
1:C:405:ALA:O	1:C:436:THR:HB	2.18	0.43
2:B:40:ASN:HA	2:B:41:PRO:HD3	1.78	0.43
2:D:119:GLN:NE2	2:D:122:THR:HG23	2.33	0.43
1:C:60:MET:HE2	1:C:66:PRO:CA	2.48	0.43
1:G:473:GLU:OE1	1:G:516:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:SER:HA	1:G:321:ALA:HB1	2.01	0.43
2:D:67:ASP:HA	2:D:106:HIS:CD2	2.53	0.43
2:D:82:VAL:O	2:D:137:PHE:HB2	2.18	0.43
1:C:269:ARG:HG3	1:C:269:ARG:HH11	1.84	0.43
1:G:485:GLU:O	1:G:485:GLU:HG3	2.19	0.43
1:C:296:HIS:O	1:C:325:CYS:HB2	2.19	0.43
1:E:335:LEU:HD22	1:E:430:VAL:HG13	2.01	0.43
1:A:470:VAL:O	1:A:517:THR:HG22	2.19	0.43
1:G:226:LEU:HD23	1:G:226:LEU:HA	1.89	0.43
1:C:60:MET:HE2	1:C:66:PRO:HA	1.99	0.43
1:A:473:GLU:HG2	1:A:516:ARG:NH1	2.34	0.43
1:G:294:PRO:CG	1:G:322:SER:CA	2.75	0.43
1:E:317:ASP:C	1:E:319:ASP:N	2.71	0.43
1:C:235:ASN:HA	1:C:236:ASN:HA	1.80	0.43
1:C:175:PRO:HB3	1:C:221:ALA:HB1	2.00	0.43
1:E:360:ILE:HG13	1:E:360:ILE:H	1.57	0.43
2:F:122:THR:HG21	2:F:127:GLY:HA3	2.01	0.43
1:G:164:MET:O	1:G:165:LYS:CG	2.67	0.43
2:B:36:TRP:CD1	2:B:77:TYR:CE2	3.07	0.43
1:C:76:MET:HG3	1:C:114:VAL:HG12	2.00	0.42
1:G:162:ARG:HH22	2:H:128:PHE:HZ	1.64	0.42
2:F:159:ARG:HG2	2:F:159:ARG:H	1.35	0.42
2:D:78:VAL:HG12	2:D:80:TYR:CE1	2.54	0.42
2:F:75:GLU:HB3	2:F:77:TYR:CE2	2.54	0.42
1:G:98:TYR:CE1	1:G:202:LYS:HE3	2.53	0.42
1:C:295:PRO:CB	1:C:324:PRO:HB3	2.49	0.42
2:H:43:PHE:CG	2:H:152:LEU:HD12	2.54	0.42
1:C:192:ILE:CG1	1:C:193:ALA:N	2.82	0.42
1:C:140:ASN:OD1	1:C:141:GLN:HG3	2.19	0.42
1:G:281:TYR:CD2	1:G:321:ALA:HB3	2.54	0.42
1:E:342:THR:HG23	1:E:403:LEU:HD12	2.01	0.42
1:C:62:GLU:OE1	1:C:63:LYS:HG3	2.19	0.42
2:F:73:LYS:HZ1	2:F:73:LYS:HA	1.85	0.42
1:G:340:ASN:CG	1:G:341:GLU:N	2.73	0.42
2:D:73:LYS:HD3	2:D:73:LYS:HA	1.87	0.42
1:G:235:ASN:HA	1:G:236:ASN:HA	1.79	0.42
1:G:298:TYR:O	1:G:307:CYS:CA	2.67	0.42
2:F:40:ASN:HA	2:F:41:PRO:HD3	1.83	0.42
1:E:164:MET:HG3	2:F:125:SER:OG	2.20	0.42
2:B:32:TYR:CD2	2:B:32:TYR:N	2.87	0.42
2:F:28:VAL:HG12	2:F:29:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:ASP:N	1:G:374:PRO:CD	2.83	0.42
2:D:70:PRO:C	2:D:72:ASP:H	2.23	0.42
1:G:138:ARG:HD3	1:G:141:GLN:HB2	2.00	0.42
2:H:131:ARG:HB2	2:H:134:ARG:HD3	2.01	0.42
1:E:373:ASP:HB3	1:E:376:LYS:HG3	2.01	0.42
1:A:348:TRP:CD1	1:A:396:THR:HG22	2.55	0.42
1:C:62:GLU:HB3	1:C:164:MET:HE1	2.02	0.42
1:A:360:ILE:HA	1:A:416:VAL:O	2.19	0.42
1:G:294:PRO:CB	1:G:322:SER:O	2.61	0.42
1:A:115:MET:C	1:E:115:MET:HB2	2.38	0.42
1:E:207:THR:HG21	1:E:253:TRP:CD1	2.55	0.42
1:E:312:GLY:O	1:E:327:ARG:NE	2.51	0.42
2:D:95:LYS:HD3	2:D:95:LYS:HA	1.66	0.42
1:C:117:THR:CA	1:G:115:MET:SD	3.03	0.41
1:C:226:LEU:CD1	1:G:254:LEU:HD13	2.50	0.41
1:A:254:LEU:HD13	1:E:226:LEU:HD12	2.02	0.41
2:F:87:TYR:CE1	2:F:153:LYS:HB2	2.54	0.41
1:A:282:LYS:HE3	1:A:287:ASP:O	2.19	0.41
1:A:419:VAL:C	1:A:421:LYS:H	2.23	0.41
2:H:65:TYR:HE2	2:H:74:THR:OG1	2.03	0.41
2:B:146:ASN:HD22	2:B:148:ARG:NH2	2.19	0.41
1:C:320:ALA:C	1:C:322:SER:N	2.73	0.41
1:A:326:THR:HG21	1:A:357:ARG:HE	1.85	0.41
1:E:317:ASP:C	1:E:319:ASP:H	2.23	0.41
2:D:125:SER:C	2:D:126:LEU:HD23	2.41	0.41
2:B:159:ARG:HH11	2:B:159:ARG:HG2	1.85	0.41
1:A:354:THR:HG23	1:A:356:GLY:CA	2.47	0.41
1:A:512:HIS:CE1	1:A:527:PRO:HG3	2.55	0.41
1:A:117:THR:OG1	1:E:115:MET:HE1	2.19	0.41
1:C:341:GLU:O	1:C:436:THR:HG22	2.18	0.41
1:G:471:ILE:HA	1:G:517:THR:HG22	2.02	0.41
1:A:236:ASN:OD1	1:A:236:ASN:N	2.53	0.41
2:F:45:ARG:HB2	2:F:45:ARG:CZ	2.51	0.41
1:C:116:GLY:C	1:G:115:MET:CG	2.88	0.41
1:G:335:LEU:HD11	1:G:346:LEU:CG	2.50	0.41
1:C:320:ALA:C	1:C:322:SER:H	2.23	0.41
1:G:354:THR:C	1:G:356:GLY:HA2	2.40	0.41
1:C:403:LEU:HB2	1:C:409:TYR:OH	2.19	0.41
1:A:357:ARG:HH12	1:A:418:GLY:HA3	1.85	0.41
1:E:129:SER:HB2	1:E:138:ARG:HH22	1.85	0.41
1:C:414:TRP:CH2	1:C:426:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:514:ARG:HD2	1:E:524:PHE:CZ	2.56	0.41
1:C:102:LYS:HA	1:C:167:ASN:O	2.20	0.41
1:G:306:SER:HA	1:G:321:ALA:CB	2.50	0.41
1:E:385:HIS:HA	1:E:386:TYR:CB	2.19	0.41
1:E:67:ILE:HG22	1:E:68:ARG:C	2.41	0.41
2:B:77:TYR:HB3	2:B:142:ALA:HA	2.02	0.41
2:B:31:ARG:HH11	2:B:31:ARG:HD3	1.75	0.41
1:A:164:MET:HE3	1:A:166:LEU:HD22	2.03	0.41
1:C:118:CYS:CA	1:G:115:MET:CE	2.97	0.41
1:E:56:GLU:HA	1:E:69:THR:O	2.20	0.41
1:E:328:PRO:HB3	1:E:420:SER:HB2	2.03	0.41
2:H:31:ARG:HG2	2:H:57:TYR:HB2	2.03	0.41
2:H:149:ARG:O	2:H:150:SER:HB3	2.21	0.41
2:H:162:ASN:O	2:H:165:MET:HG2	2.21	0.41
1:G:237:SER:HB3	1:G:273:CYS:SG	2.61	0.41
1:A:96:ARG:HE	1:A:96:ARG:HB2	1.56	0.41
2:H:74:THR:O	2:H:76:ARG:NH1	2.54	0.41
1:A:357:ARG:HH12	1:A:418:GLY:H	1.69	0.41
2:H:82:VAL:HG12	2:H:96:GLY:HA3	2.02	0.41
2:H:40:ASN:HA	2:H:41:PRO:HD2	1.84	0.41
1:C:282:LYS:HE3	1:C:287:ASP:O	2.21	0.41
2:H:119:GLN:HE22	2:H:122:THR:HG22	1.78	0.41
1:C:436:THR:HG22	1:C:437:ASN:N	2.34	0.41
1:E:320:ALA:O	1:E:322:SER:N	2.54	0.41
1:E:362:TYR:HA	1:E:414:TRP:O	2.20	0.41
1:G:106:ARG:HD2	1:G:154:PHE:CZ	2.56	0.41
1:G:59:ILE:O	1:G:67:ILE:N	2.49	0.40
1:A:61:ASP:OD2	1:A:67:ILE:CD1	2.68	0.40
2:D:54:ILE:HD12	2:D:132:PRO:HG3	2.01	0.40
2:D:31:ARG:HD3	2:D:59:ASP:OD2	2.22	0.40
2:D:104:ARG:HH22	2:D:108:PRO:HD3	1.86	0.40
1:G:386:TYR:CZ	1:G:390:GLN:HG3	2.55	0.40
2:H:78:VAL:HG22	2:H:101:GLU:HG2	2.02	0.40
1:C:455:TYR:CE2	1:C:540:ILE:HD12	2.56	0.40
1:C:296:HIS:CB	1:C:325:CYS:HB2	2.50	0.40
2:F:104:ARG:HB3	2:F:107:SER:HB3	2.03	0.40
2:H:49:HIS:HA	2:H:155:LYS:O	2.21	0.40
1:G:438:GLN:HB3	1:G:468:ASN:O	2.21	0.40
1:E:59:ILE:HD12	1:E:69:THR:HG21	2.04	0.40
1:G:254:LEU:HA	1:G:254:LEU:HD23	1.79	0.40
2:B:32:TYR:CD2	2:B:52:VAL:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:CYS:SG	1:A:367:LYS:N	2.94	0.40
2:F:154:LEU:HD12	2:F:154:LEU:HA	1.83	0.40
1:G:91:ARG:NE	1:G:178:LYS:O	2.51	0.40
1:E:471:ILE:HA	1:E:517:THR:HG22	2.03	0.40
2:D:120:LEU:HD23	2:D:120:LEU:HA	1.89	0.40
2:D:40:ASN:HA	2:D:41:PRO:HD3	1.92	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:ILE:O	1:G:266:HIS:NE2[2_464]	1.99	0.21

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	514/518 (99%)	473 (92%)	38 (7%)	3 (1%)	30	70
1	C	514/518 (99%)	475 (92%)	35 (7%)	4 (1%)	24	64
1	E	514/518 (99%)	481 (94%)	29 (6%)	4 (1%)	24	64
1	G	514/518 (99%)	479 (93%)	30 (6%)	5 (1%)	19	59
2	B	139/141 (99%)	120 (86%)	17 (12%)	2 (1%)	14	50
2	D	138/141 (98%)	122 (88%)	14 (10%)	2 (1%)	14	50
2	F	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	26	67
2	H	136/141 (96%)	121 (89%)	10 (7%)	5 (4%)	4	24
All	All	2605/2636 (99%)	2393 (92%)	186 (7%)	26 (1%)	19	59

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	ASP
1	G	62	GLU
1	G	164	MET
1	G	165	LYS
2	B	103	ASN
1	E	41	GLY
2	H	145	ASP
1	A	390	GLN
2	B	88	SER
1	E	377	CYS
1	E	419	VAL
2	H	164	CYS
1	A	419	VAL
2	D	47	ASP
2	D	146	ASN
1	E	405	ALA
2	H	39	SER
2	H	150	SER
1	A	375	SER
1	C	41	GLY
1	C	382	SER
2	F	90	CYS
1	G	334	ASN
2	H	108	PRO
1	G	419	VAL
1	C	419	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/447 (100%)	414 (93%)	33 (7%)	17	51
1	C	447/447 (100%)	410 (92%)	37 (8%)	14	46
1	E	447/447 (100%)	414 (93%)	33 (7%)	17	51
1	G	447/447 (100%)	418 (94%)	29 (6%)	21	57
2	B	127/127 (100%)	116 (91%)	11 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	127/127 (100%)	114 (90%)	13 (10%)	9 33
2	F	127/127 (100%)	114 (90%)	13 (10%)	9 33
2	H	127/127 (100%)	114 (90%)	13 (10%)	9 33
All	All	2296/2296 (100%)	2114 (92%)	182 (8%)	15 48

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	67	ILE
1	A	76	MET
1	A	90	THR
1	A	105	LEU
1	A	107	ASP
1	A	119	LYS
1	A	120	GLU
1	A	143	VAL
1	A	192	ILE
1	A	206	LEU
1	A	236	ASN
1	A	270	SER
1	A	317	ASP
1	A	327	ARG
1	A	336	ILE
1	A	340	ASN
1	A	346	LEU
1	A	357	ARG
1	A	360	ILE
1	A	366	CYS
1	A	369	CYS
1	A	380	CYS
1	A	385	HIS
1	A	387	THR
1	A	395	THR
1	A	396	THR
1	A	404	LEU
1	A	436	THR
1	A	466	ARG
1	A	483	GLN
1	A	506	LEU
1	A	514	ARG

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Mol	Chain	Res	Type
2	B	31	ARG
2	B	38	SER
2	B	42	ARG
2	B	48	TYR
2	B	74	THR
2	B	79	LEU
2	B	104	ARG
2	B	122	THR
2	B	125	SER
2	B	141	SER
2	B	165	MET
1	C	38	SER
1	C	62	GLU
1	C	67	ILE
1	C	68	ARG
1	C	107	ASP
1	C	119	LYS
1	C	120	GLU
1	C	139	GLU
1	C	143	VAL
1	C	192	ILE
1	C	206	LEU
1	C	232	SER
1	C	236	ASN
1	C	270	SER
1	C	300	VAL
1	C	317	ASP
1	C	318	ASN
1	C	327	ARG
1	C	336	ILE
1	C	338	ASN
1	C	339	VAL
1	C	357	ARG
1	C	360	ILE
1	C	366	CYS
1	C	367	LYS
1	C	369	CYS
1	C	373	ASP
1	C	378	ARG
1	C	380	CYS
1	C	387	THR
1	C	393	LEU

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Mol	Chain	Res	Type
1	C	395	THR
1	C	402	ASP
1	C	466	ARG
1	C	483	GLN
1	C	506	LEU
1	C	514	ARG
2	D	42	ARG
2	D	48	TYR
2	D	79	LEU
2	D	85	ASP
2	D	91	ASP
2	D	122	THR
2	D	125	SER
2	D	134	ARG
2	D	149	ARG
2	D	155	LYS
2	D	161	THR
2	D	163	SER
2	D	165	MET
1	E	43	LEU
1	E	46	ILE
1	E	105	LEU
1	E	107	ASP
1	E	115	MET
1	E	119	LYS
1	E	120	GLU
1	E	139	GLU
1	E	143	VAL
1	E	187	ASP
1	E	192	ILE
1	E	206	LEU
1	E	236	ASN
1	E	270	SER
1	E	311	ARG
1	E	315	ARG
1	E	317	ASP
1	E	318	ASN
1	E	340	ASN
1	E	357	ARG
1	E	360	ILE
1	E	369	CYS
1	E	380	CYS

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Mol	Chain	Res	Type
1	E	385	HIS
1	E	387	THR
1	E	395	THR
1	E	396	THR
1	E	436	THR
1	E	465	ASP
1	E	466	ARG
1	E	483	GLN
1	E	506	LEU
1	E	514	ARG
2	F	30	ASP
2	F	45	ARG
2	F	48	TYR
2	F	54	ILE
2	F	79	LEU
2	F	85	ASP
2	F	93	THR
2	F	103	ASN
2	F	122	THR
2	F	151	CYS
2	F	159	ARG
2	F	162	ASN
2	F	163	SER
1	G	68	ARG
1	G	90	THR
1	G	105	LEU
1	G	107	ASP
1	G	115	MET
1	G	120	GLU
1	G	126	TYR
1	G	143	VAL
1	G	192	ILE
1	G	206	LEU
1	G	236	ASN
1	G	278	ILE
1	G	307	CYS
1	G	317	ASP
1	G	327	ARG
1	G	357	ARG
1	G	360	ILE
1	G	366	CYS
1	G	376	LYS

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Mol	Chain	Res	Type
1	G	385	HIS
1	G	387	THR
1	G	393	LEU
1	G	395	THR
1	G	416	VAL
1	G	438	GLN
1	G	466	ARG
1	G	483	GLN
1	G	506	LEU
1	G	514	ARG
2	H	38	SER
2	H	44	GLN
2	H	48	TYR
2	H	72	ASP
2	H	73	LYS
2	H	79	LEU
2	H	91	ASP
2	H	93	THR
2	H	104	ARG
2	H	125	SER
2	H	143	ILE
2	H	152	LEU
2	H	159	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	HIS
2	B	83	ASN
2	B	146	ASN
1	E	437	ASN
1	E	438	GLN
1	G	71	GLN
1	G	345	ASN
2	H	119	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 carbohydrates are modelled in this entry.

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	$\#\|Z\|>2$
4	NAG	A	3402	1,4	14,14,15	0.79	1 (7%)	15,19,21	2.82	2 (13%)
4	NAG	A	3403	4	14,14,15	0.47	0	15,19,21	1.12	1 (6%)
4	NAG	B	201	2,4	14,14,15	0.45	0	15,19,21	2.23	5 (33%)
4	NAG	B	202	4	14,14,15	0.58	0	15,19,21	1.62	2 (13%)
4	NAG	C	601	1,4	14,14,15	0.53	0	15,19,21	0.89	0
4	NAG	C	602	4	14,14,15	0.51	0	15,19,21	2.00	3 (20%)
4	NAG	D	201	2,4	14,14,15	0.91	1 (7%)	15,19,21	1.93	4 (26%)
4	NAG	D	202	4	14,14,15	0.53	0	15,19,21	1.47	3 (20%)
4	NAG	E	3402	1,4	14,14,15	0.59	0	15,19,21	2.67	7 (46%)
4	NAG	E	3403	4	14,14,15	0.61	0	15,19,21	1.86	4 (26%)
4	NAG	F	201	2,4	14,14,15	0.50	0	15,19,21	1.88	5 (33%)
4	NAG	F	202	4	14,14,15	0.48	0	15,19,21	1.13	1 (6%)
4	NAG	G	3402	1,4	14,14,15	0.42	0	15,19,21	1.55	2 (13%)
4	NAG	G	3403	4	14,14,15	0.50	0	15,19,21	1.46	2 (13%)
4	NAG	H	201	2,4	14,14,15	0.99	1 (7%)	15,19,21	2.02	5 (33%)
4	NAG	H	202	4	14,14,15	0.60	0	15,19,21	1.04	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
4	NAG	A	3402	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3403	4	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	4	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	602	4	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	202	4	-	0/6/23/26	0/1/1/1
4	NAG	E	3402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	3403	4	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	202	4	-	0/6/23/26	0/1/1/1
4	NAG	G	3402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	3403	4	-	0/6/23/26	0/1/1/1
4	NAG	H	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	202	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	NAG	O5-C1	-2.79	1.39	1.43
4	A	3402	NAG	C1-C2	2.39	1.55	1.52
4	H	201	NAG	O7-C7	2.45	1.28	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	201	NAG	C1-O5-C5	-4.77	106.19	112.25
4	D	201	NAG	C2-N2-C7	-4.65	117.06	123.04
4	H	201	NAG	C2-N2-C7	-4.05	117.84	123.04
4	B	201	NAG	C3-C4-C5	-3.58	103.96	110.20
4	D	201	NAG	C3-C4-C5	-3.46	104.16	110.20
4	B	202	NAG	C3-C4-C5	-3.36	104.34	110.20
4	E	3402	NAG	O7-C7-C8	-2.89	116.76	122.06
4	D	201	NAG	C1-O5-C5	-2.71	108.81	112.25
4	F	201	NAG	C3-C4-C5	-2.56	105.73	110.20
4	E	3403	NAG	O7-C7-C8	-2.47	117.52	122.06
4	H	201	NAG	C8-C7-N2	-2.22	111.86	116.11
4	F	201	NAG	C3-C2-N2	-2.19	105.31	110.56
4	D	202	NAG	O7-C7-C8	-2.08	118.25	122.06
4	B	201	NAG	C3-C2-N2	-2.06	105.63	110.56
4	D	202	NAG	O7-C7-N2	2.04	126.03	121.86
4	G	3402	NAG	O4-C4-C5	2.08	114.75	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	201	NAG	O7-C7-N2	2.15	126.25	121.86
4	G	3403	NAG	C2-N2-C7	2.20	125.87	123.04
4	H	201	NAG	O5-C5-C6	2.22	112.16	107.35
4	D	201	NAG	C3-C2-N2	2.25	115.94	110.56
4	B	202	NAG	C3-C2-N2	2.27	116.00	110.56
4	B	201	NAG	O7-C7-N2	2.43	126.82	121.86
4	E	3403	NAG	C1-O5-C5	2.46	115.37	112.25
4	E	3402	NAG	C3-C2-N2	2.46	116.46	110.56
4	H	201	NAG	O7-C7-N2	2.50	126.95	121.86
4	F	202	NAG	C1-O5-C5	2.51	115.44	112.25
4	A	3403	NAG	C1-O5-C5	2.52	115.44	112.25
4	A	3402	NAG	O4-C4-C5	2.59	116.10	109.24
4	E	3402	NAG	C4-C3-C2	2.64	115.33	111.23
4	E	3402	NAG	C3-C4-C5	2.69	114.89	110.20
4	E	3402	NAG	C1-O5-C5	2.77	115.76	112.25
4	E	3403	NAG	C8-C7-N2	2.93	121.71	116.11
4	C	602	NAG	C8-C7-N2	2.93	121.71	116.11
4	E	3402	NAG	C8-C7-N2	3.12	122.07	116.11
4	F	201	NAG	O5-C5-C6	3.16	114.18	107.35
4	B	201	NAG	O5-C5-C6	3.23	114.34	107.35
4	D	202	NAG	O3-C3-C2	3.30	115.64	109.11
4	G	3403	NAG	C1-O5-C5	3.99	117.31	112.25
4	C	602	NAG	C1-O5-C5	4.23	117.62	112.25
4	F	201	NAG	C2-N2-C7	4.53	128.86	123.04
4	G	3402	NAG	C1-O5-C5	4.64	118.13	112.25
4	C	602	NAG	C2-N2-C7	4.72	129.11	123.04
4	E	3403	NAG	C2-N2-C7	5.29	129.84	123.04
4	B	201	NAG	C2-N2-C7	5.79	130.48	123.04
4	E	3402	NAG	C2-N2-C7	7.50	132.68	123.04
4	A	3402	NAG	C1-O5-C5	10.22	125.22	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	601	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	NAG	1	0
4	D	201	NAG	1	0
4	E	3402	NAG	2	0
4	E	3403	NAG	1	0
4	G	3402	NAG	1	0
4	H	201	NAG	3	0

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	3401	1	14,14,15	0.48	0	15,19,21	1.29	2 (13%)
3	NAG	E	3401	1	14,14,15	0.49	0	15,19,21	2.16	1 (6%)
3	NAG	G	3401	1	14,14,15	0.54	0	15,19,21	2.04	1 (6%)

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	NAG	A	3401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	3401	1	-	0/6/23/26	0/1/1/1
3	NAG	G	3401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3401	NAG	O5-C5-C6	2.11	111.93	107.35
3	A	3401	NAG	C1-O5-C5	3.59	116.80	112.25
3	G	3401	NAG	C1-O5-C5	7.12	121.29	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3401	NAG	C1-O5-C5	7.96	122.35	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	516/518 (99%)	0.34	39 (7%) 17 6	63, 154, 346, 442	0
1	C	516/518 (99%)	-0.07	24 (4%) 35 16	59, 111, 216, 263	0
1	E	516/518 (99%)	0.41	46 (8%) 12 4	65, 161, 327, 484	0
1	G	516/518 (99%)	0.41	43 (8%) 14 5	74, 168, 265, 356	0
2	B	141/141 (100%)	-0.32	2 (1%) 78 61	52, 94, 187, 261	0
2	D	140/141 (99%)	-0.30	3 (2%) 67 46	55, 91, 177, 216	0
2	F	138/141 (97%)	-0.33	1 (0%) 89 79	66, 112, 200, 262	0
2	H	138/141 (97%)	-0.14	8 (5%) 26 10	82, 124, 238, 270	0
All	All	2621/2636 (99%)	0.16	166 (6%) 23 9	52, 135, 274, 484	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	537	SER	16.4
1	G	537	SER	15.1
1	E	541	GLY	14.3
1	G	540	ILE	12.6
1	G	322	SER	10.7
1	E	536	PRO	10.5
1	E	538	ARG	10.2
1	E	542	ASP	8.6
1	G	485	GLU	8.3
1	G	321	ALA	8.3
1	C	538	ARG	8.1
1	G	541	GLY	7.8
1	G	114	VAL	6.9
1	E	421	LYS	6.8
1	G	484	ASN	6.8
1	G	538	ARG	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	42	GLU	6.5
1	E	422	TYR	6.2
1	G	539	ILE	6.1
1	E	512	HIS	5.8
1	E	449	ALA	5.7
1	E	534	THR	5.4
1	E	42	GLU	5.4
1	G	383	GLY	5.4
1	C	537	SER	5.3
1	E	479	TYR	5.1
1	A	449	ALA	5.1
1	E	529	GLU	5.0
1	E	458	ALA	4.9
1	G	341	GLU	4.8
1	G	536	PRO	4.8
1	C	135	ARG	4.8
1	A	482	ASP	4.7
1	A	487	SER	4.6
1	A	317	ASP	4.5
1	E	372	GLY	4.4
1	G	487	SER	4.4
1	C	153	SER	4.3
1	E	373	ASP	4.2
1	A	542	ASP	4.2
1	E	465	ASP	4.2
1	E	487	SER	4.2
1	E	539	ILE	4.2
1	E	66	PRO	4.2
1	A	318	ASN	4.2
1	C	540	ILE	4.2
1	G	312	GLY	4.1
1	G	542	ASP	4.1
1	A	153	SER	4.1
1	C	541	GLY	4.1
1	E	485	GLU	4.1
1	G	324	PRO	4.0
1	G	115	MET	4.0
1	G	58	SER	3.9
1	E	540	ILE	3.9
1	G	314	PHE	3.9
1	E	511	PHE	3.8
1	A	486	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	462	LEU	3.8
1	E	455	TYR	3.8
1	C	373	ASP	3.7
1	A	418	GLY	3.6
1	A	483	GLN	3.5
1	A	538	ARG	3.5
1	A	535	VAL	3.5
2	H	146	ASN	3.5
1	A	136	PHE	3.5
1	C	277	LYS	3.5
1	A	509	TYR	3.5
1	C	536	PRO	3.4
1	E	535	VAL	3.4
1	G	319	ASP	3.4
1	G	488	TYR	3.3
1	E	480	GLU	3.3
1	G	78	PRO	3.3
1	E	114	VAL	3.3
1	A	484	ASN	3.3
1	E	484	ASN	3.2
1	A	541	GLY	3.2
1	G	535	VAL	3.2
1	C	136	PHE	3.2
1	E	475	GLU	3.1
1	C	27	PRO	3.1
1	G	295	PRO	3.1
1	G	42	GLU	3.1
1	A	297	SER	3.1
1	G	325	CYS	3.1
1	E	460	ALA	3.1
1	E	418	GLY	3.1
1	A	358	GLN	3.1
2	D	148	ARG	3.1
2	H	73	LYS	3.0
2	H	145	ASP	3.0
1	A	485	GLU	3.0
2	H	148	ARG	2.9
1	A	458	ALA	2.9
1	G	66	PRO	2.9
1	C	449	ALA	2.9
1	A	501	LYS	2.8
1	A	499	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	274	GLN	2.8
1	A	502	GLY	2.8
1	E	385	HIS	2.8
1	E	444	ILE	2.8
1	A	539	ILE	2.8
1	C	534	THR	2.8
1	A	451	GLU	2.7
1	G	301	TRP	2.7
1	E	513	VAL	2.7
1	A	480	GLU	2.7
1	C	484	ASN	2.7
2	D	146	ASN	2.7
1	C	58	SER	2.6
1	G	116	GLY	2.6
1	G	480	GLU	2.6
1	A	58	SER	2.6
1	A	152	GLU	2.6
1	E	486	ARG	2.6
2	H	68	SER	2.6
2	D	94	SER	2.6
1	E	459	LEU	2.5
1	C	154	PHE	2.5
1	G	323	MET	2.5
1	A	135	ARG	2.5
1	G	68	ARG	2.5
1	A	536	PRO	2.5
1	A	154	PHE	2.5
1	C	508	SER	2.5
1	E	27	PRO	2.5
1	C	542	ASP	2.4
1	G	127	TYR	2.4
1	G	486	ARG	2.4
1	G	530	VAL	2.4
1	A	492	ARG	2.4
1	E	370	GLY	2.4
1	A	78	PRO	2.4
1	G	153	SER	2.3
1	G	61	ASP	2.3
1	C	65	THR	2.3
2	B	26	ALA	2.3
1	E	292	LYS	2.3
2	H	144	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	330	SER	2.3
1	E	58	SER	2.3
1	C	298	TYR	2.3
1	G	240	LYS	2.2
1	C	152	GLU	2.2
1	G	511	PHE	2.2
1	G	519	ALA	2.2
1	C	66	PRO	2.2
2	H	66	GLU	2.2
1	A	295	PRO	2.2
1	A	370	GLY	2.2
1	E	59	ILE	2.2
1	E	387	THR	2.1
1	A	296	HIS	2.1
1	G	296	HIS	2.1
2	H	106	HIS	2.1
1	A	375	SER	2.1
1	E	65	THR	2.1
2	B	71	GLU	2.1
1	G	292	LYS	2.1
2	F	28	VAL	2.1
1	E	153	SER	2.0
1	A	488	TYR	2.0
1	C	452	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	G	3402	14/15	0.87	0.29	0.43	194,202,215,218	0
4	NAG	E	3402	14/15	0.88	0.19	-0.47	197,221,234,235	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	D	201	14/15	0.95	0.14	-0.62	79,85,98,117	0
4	NAG	H	201	14/15	0.95	0.14	-0.76	92,105,139,142	0
4	NAG	A	3402	14/15	0.84	0.27	-0.93	215,228,236,249	0
4	NAG	B	201	14/15	0.97	0.10	-1.00	76,86,96,100	0
4	NAG	F	201	14/15	0.97	0.10	-1.38	97,105,116,122	0
4	NAG	C	602	14/15	0.77	0.51	-	162,181,188,207	0
4	NAG	A	3403	14/15	0.86	0.44	-	267,281,301,301	0
4	NAG	F	202	14/15	0.88	0.14	-	126,136,149,161	0
4	NAG	B	202	14/15	0.89	0.18	-	94,101,126,127	0
4	NAG	H	202	14/15	0.91	0.24	-	114,124,156,161	0
4	NAG	C	601	14/15	0.96	0.13	-	112,127,154,169	0
4	NAG	G	3403	14/15	0.86	0.23	-	186,213,229,232	0
4	NAG	E	3403	14/15	0.85	0.30	-	203,226,238,248	0
4	NAG	D	202	14/15	0.94	0.15	-	96,100,112,113	0

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	E	3401	14/15	0.38	0.31	0.39	207,252,264,265	0
3	NAG	G	3401	14/15	0.58	0.29	-	210,231,255,273	0
3	NAG	A	3401	14/15	0.55	0.30	-	195,227,234,236	0

6.5 Other polymers (i)

There are no such residues in this entry.