Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:13 PM GMT

PDB ID	:	4KWM
Title	:	Structure of a/anhui/5/2005 h5 ha
Authors	:	Yang, H.; Shore, D.A.; Carney, P.J.; Chang, J.C.; Stevens, J.
Deposited on	:	2013-05-24
Resolution	:	2.70 Å(reported)

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

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

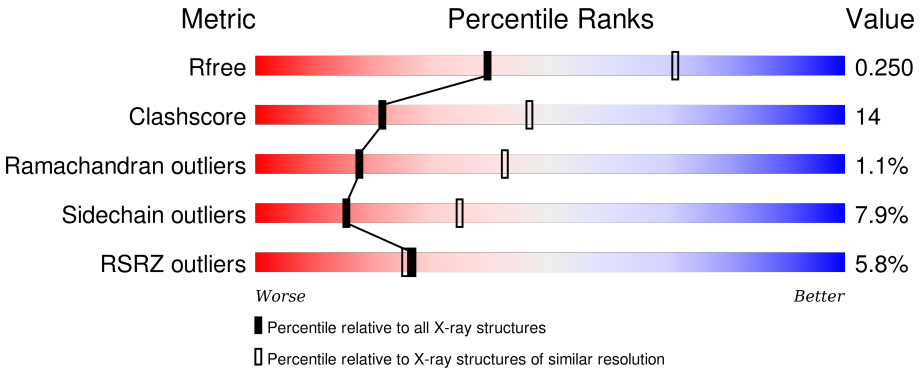
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	329	2% 71% 22%
1	C	329	68% 25% 5%
1	E	329	7% 66% 27% 5%
2	B	174	2% 66% 26% 6%
2	D	174	65% 26% 6%

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Mol	Chain	Length	Quality of chain
2	F	174	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	401	X	-	-	-
3	NAG	B	201	X	-	-	-
3	NAG	D	201	X	-	-	-
3	NAG	E	401	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11879 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2548	1610	438	487	13			
1	C	322	Total	C	N	O	S	0	0	0
			2541	1605	437	486	13			
1	E	322	Total	C	N	O	S	0	0	0
			2541	1605	437	486	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	EXPRESSION TAG	UNP C0LYC6
A	-2	ASP	-	EXPRESSION TAG	UNP C0LYC6
A	-1	PRO	-	EXPRESSION TAG	UNP C0LYC6
A	0	GLY	-	EXPRESSION TAG	UNP C0LYC6
A	151	ILE	THR	CONFLICT	UNP C0LYC6
A	171	ASP	ASN	CONFLICT	UNP C0LYC6
A	188	THR	ILE	CONFLICT	UNP C0LYC6
A	259	LYS	GLU	CONFLICT	UNP C0LYC6
A	265	VAL	MET	CONFLICT	UNP C0LYC6
A	273	ASN	TYR	CONFLICT	UNP C0LYC6
C	-3	ALA	-	EXPRESSION TAG	UNP C0LYC6
C	-2	ASP	-	EXPRESSION TAG	UNP C0LYC6
C	-1	PRO	-	EXPRESSION TAG	UNP C0LYC6
C	0	GLY	-	EXPRESSION TAG	UNP C0LYC6
C	151	ILE	THR	CONFLICT	UNP C0LYC6
C	171	ASP	ASN	CONFLICT	UNP C0LYC6
C	188	THR	ILE	CONFLICT	UNP C0LYC6
C	259	LYS	GLU	CONFLICT	UNP C0LYC6
C	265	VAL	MET	CONFLICT	UNP C0LYC6
C	273	ASN	TYR	CONFLICT	UNP C0LYC6
E	-3	ALA	-	EXPRESSION TAG	UNP C0LYC6
E	-2	ASP	-	EXPRESSION TAG	UNP C0LYC6
E	-1	PRO	-	EXPRESSION TAG	UNP C0LYC6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	EXPRESSION TAG	UNP C0LYC6
E	151	ILE	THR	CONFLICT	UNP C0LYC6
E	171	ASP	ASN	CONFLICT	UNP C0LYC6
E	188	THR	ILE	CONFLICT	UNP C0LYC6
E	259	LYS	GLU	CONFLICT	UNP C0LYC6
E	265	VAL	MET	CONFLICT	UNP C0LYC6
E	273	ASN	TYR	CONFLICT	UNP C0LYC6

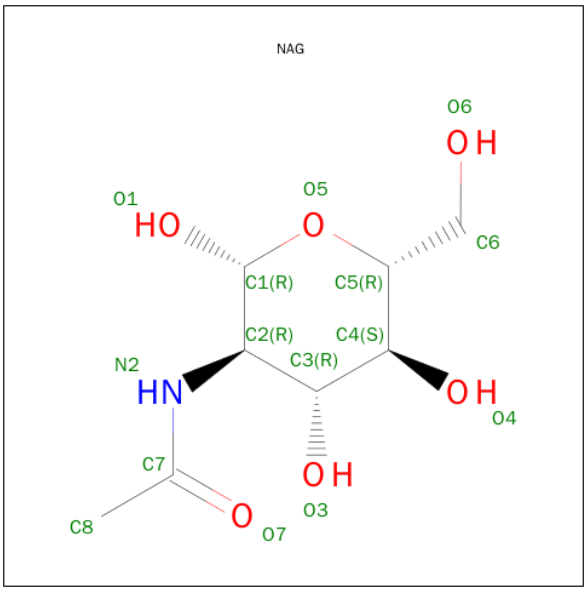
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1346	833	235	270	8			
2	D	164	Total	C	N	O	S	0	0	0
			1346	833	235	270	8			
2	F	164	Total	C	N	O	S	0	0	0
			1346	833	235	270	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	GLU	GLY	CONFLICT	UNP C0LYC6
D	64	GLU	GLY	CONFLICT	UNP C0LYC6
F	64	GLU	GLY	CONFLICT	UNP C0LYC6

- 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 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

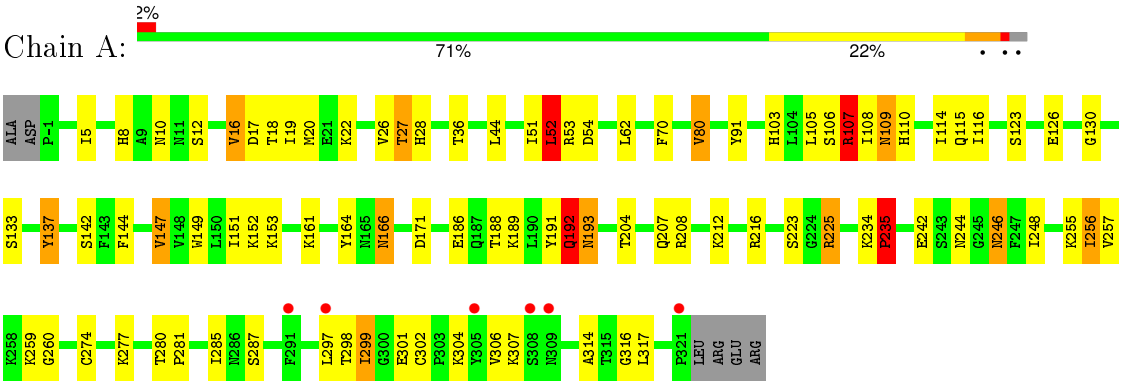
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	18	Total O 18 18	0	0
4	C	57	Total O 57 57	0	0
4	D	30	Total O 30 30	0	0
4	E	7	Total O 7 7	0	0
4	F	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

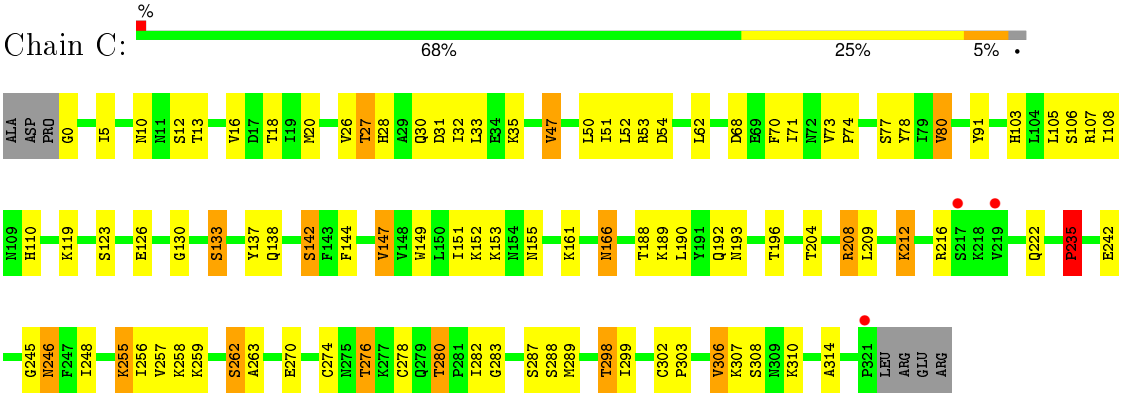
- Molecule 1: Hemagglutinin

Chain A:



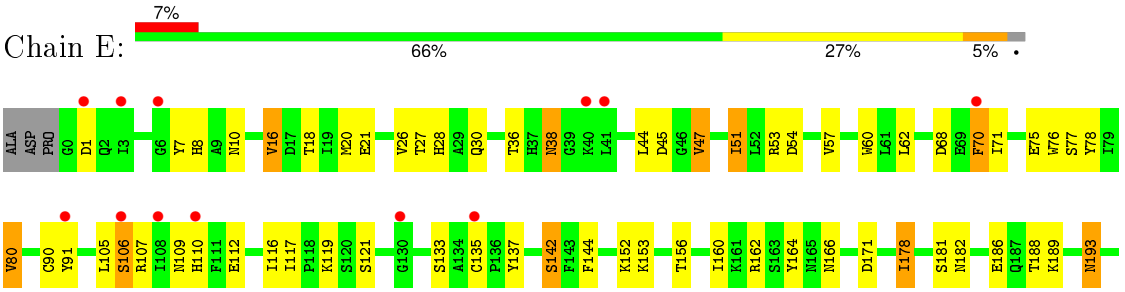
- Molecule 1: Hemagglutinin

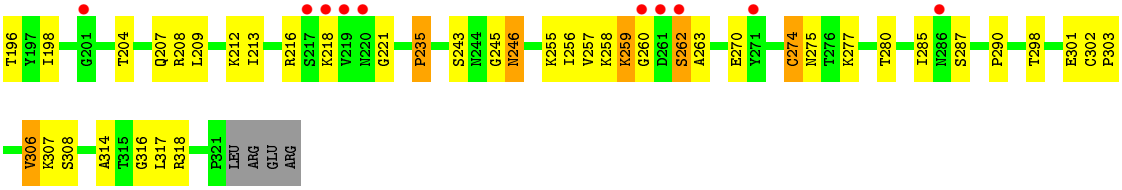
Chain C:



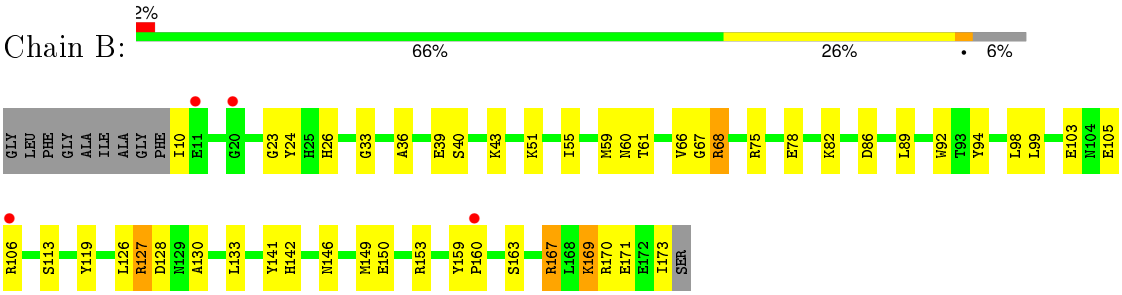
- Molecule 1: Hemagglutinin

Chain E:

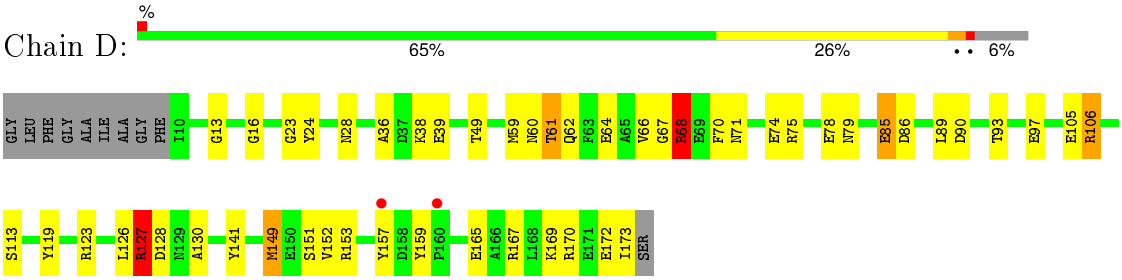




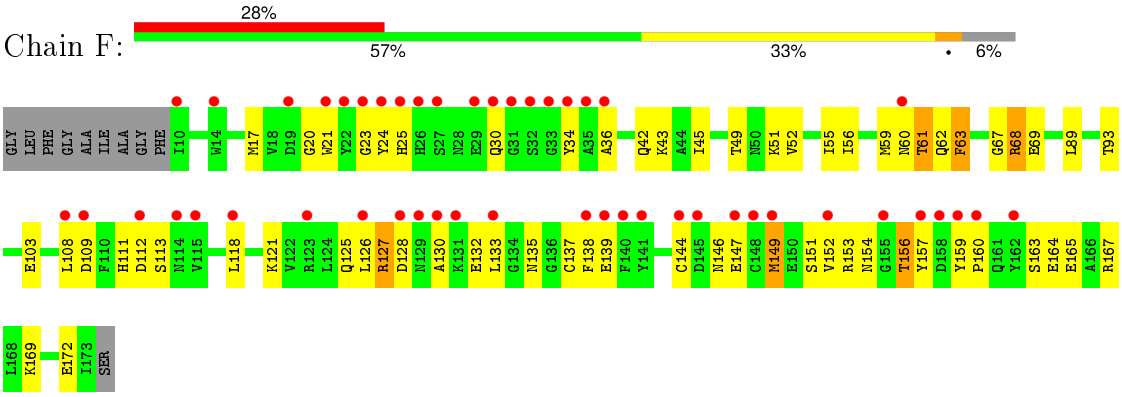
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	114.37Å 114.37Å 134.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.49 – 2.70 46.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.49-2.70) 100.0 (46.49-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.208 , 0.247 0.216 , 0.250	Depositor DCC
R_{free} test set	2834 reflections (5.51%)	DCC
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.0	EDS
Estimated twinning fraction	0.662 for H, K, L 0.338 for K, H, -L 0.000 for -h,-k,l 0.125 for h,-h-k,-l 0.006 for -k,-h,-l	Xtriage
Reported twinning fraction	0.662 for H, K, L 0.338 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 54230 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11879	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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	0.77	0/2611	0.74	2/3551 (0.1%)
1	C	0.77	0/2603	0.70	0/3540
1	E	0.54	0/2603	0.68	0/3540
2	B	0.63	0/1371	0.67	0/1843
2	D	0.78	1/1371 (0.1%)	0.69	0/1843
2	F	0.52	0/1371	0.67	0/1843
All	All	0.68	1/11930 (0.0%)	0.70	2/16160 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	85	GLU	N-CA	5.06	1.56	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	107	ARG	CG-CD-NE	5.02	122.34	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2548	0	2485	70	0
1	C	2541	0	2479	71	0
1	E	2541	0	2478	84	0
2	B	1346	0	1251	39	0
2	D	1346	0	1251	35	1
2	F	1346	0	1252	48	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
4	A	39	0	0	3	0
4	B	18	0	0	3	0
4	C	57	0	0	16	0
4	D	30	0	0	8	0
4	E	7	0	0	4	0
4	F	4	0	0	2	0
All	All	11879	0	11248	323	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 14.

All (323) 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:E:182:ASN:N	1:E:186:GLU:OE2	1.77	1.17
1:A:106:SER:O	4:A:505:HOH:O	1.75	1.02
1:A:107:ARG:HD2	1:A:260:GLY:O	1.67	0.95
1:A:103:HIS:O	1:A:106:SER:OG	1.85	0.95
2:F:51:LYS:HE2	2:F:103:GLU:HG3	1.49	0.94
1:E:70:PHE:CG	1:E:70:PHE:O	2.19	0.93
1:E:178:ILE:HD11	1:E:198:ILE:HD13	1.53	0.88
1:A:114:ILE:HD11	1:A:255:LYS:HE2	1.56	0.88
1:E:256:ILE:HB	1:E:259:LYS:HE2	1.54	0.87
1:A:17:ASP:OD2	1:A:22:LYS:HD2	1.75	0.87
2:B:141:TYR:O	2:B:169:LYS:HE3	1.76	0.84
1:A:27:THR:HG23	1:A:28:HIS:HD2	1.41	0.84
2:D:85:GLU:OE2	4:D:313:HOH:O	1.95	0.83
1:C:307:LYS:HE3	2:D:89:LEU:HD21	1.62	0.81
1:C:262:SER:O	4:C:411:HOH:O	2.00	0.79
1:E:70:PHE:CD1	1:E:70:PHE:O	2.38	0.77
2:B:170:ARG:O	2:B:173:ILE:HG22	1.85	0.77
1:A:114:ILE:HD11	1:A:255:LYS:CE	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HE3	2:B:89:LEU:HD21	1.66	0.76
2:B:160:PRO:HA	2:B:163:SER:OG	1.85	0.76
1:A:36:THR:O	1:A:285:ILE:HD13	1.86	0.76
1:A:19:ILE:HD12	1:A:20:MET:HG3	1.66	0.76
2:D:86:ASP:OD1	4:D:317:HOH:O	2.04	0.75
1:E:36:THR:O	1:E:285:ILE:HD13	1.86	0.75
1:A:304:LYS:HE2	2:B:92:TRP:CD2	2.22	0.75
1:E:77:SER:O	1:E:262:SER:HB3	1.87	0.75
2:D:59:MET:C	2:D:61:THR:H	1.90	0.75
1:C:119:LYS:NZ	4:C:440:HOH:O	2.18	0.74
2:F:154:ASN:ND2	4:F:204:HOH:O	2.18	0.74
1:C:212:LYS:O	1:C:216:ARG:NH2	2.19	0.74
1:E:258:LYS:HA	1:E:259:LYS:HZ1	1.53	0.73
1:E:178:ILE:CD1	1:E:198:ILE:HD13	2.18	0.73
1:A:27:THR:HG23	1:A:28:HIS:CD2	2.24	0.73
2:D:105:GLU:OE2	2:D:106:ARG:NH1	2.22	0.73
1:C:276:THR:HG23	1:C:278:CYS:H	1.53	0.72
1:E:7:TYR:OH	4:E:506:HOH:O	2.04	0.72
1:E:116:ILE:HD11	1:E:164:TYR:CE2	2.24	0.71
2:B:26:HIS:ND1	4:B:315:HOH:O	2.23	0.71
1:C:133:SER:O	4:C:448:HOH:O	2.08	0.71
1:C:310:LYS:O	4:C:428:HOH:O	2.08	0.70
1:C:68:ASP:OD2	1:C:71:ILE:HD11	1.91	0.70
1:E:60:TRP:NE1	1:E:70:PHE:CD1	2.60	0.70
1:A:18:THR:HG22	1:A:20:MET:H	1.57	0.69
1:C:298:THR:OG1	1:C:302:CYS:SG	2.51	0.69
1:E:109:ASN:HD21	1:E:258:LYS:HE3	1.58	0.68
1:A:171:ASP:O	1:A:256:ILE:HG23	1.93	0.68
1:A:256:ILE:HD11	1:A:259:LYS:HG3	1.76	0.68
1:C:30:GLN:NE2	4:C:455:HOH:O	2.25	0.68
2:D:64:GLU:O	4:D:301:HOH:O	2.11	0.68
2:D:123:ARG:O	4:D:314:HOH:O	2.10	0.68
1:E:75:GLU:OE2	1:E:109:ASN:ND2	2.26	0.68
2:B:33:GLY:O	4:B:315:HOH:O	2.12	0.68
1:A:256:ILE:O	1:A:256:ILE:HG13	1.93	0.68
1:C:18:THR:HG22	1:C:20:MET:H	1.58	0.68
1:A:126:GLU:HB3	1:A:151:ILE:HG13	1.74	0.68
1:C:270:GLU:OE2	4:C:426:HOH:O	2.11	0.67
1:E:1:ASP:OD2	2:F:144:CYS:N	2.22	0.66
1:E:18:THR:HG22	1:E:20:MET:H	1.59	0.66
1:E:106:SER:O	1:E:262:SER:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:THR:HB	1:C:245:GLY:HA3	1.77	0.66
2:F:156:THR:O	2:F:156:THR:OG1	2.08	0.66
2:F:126:LEU:HD13	2:F:130:ALA:HB3	1.76	0.66
1:C:276:THR:HG21	1:C:278:CYS:O	1.95	0.65
1:E:16:VAL:HG11	1:E:314:ALA:HB2	1.77	0.65
1:A:304:LYS:HD2	2:B:59:MET:CE	2.27	0.65
2:D:16:GLY:N	4:D:312:HOH:O	2.25	0.64
1:A:16:VAL:HG11	1:A:314:ALA:HB2	1.79	0.64
1:C:161:LYS:HG2	1:C:242:GLU:HG3	1.79	0.64
1:E:193:ASN:N	4:E:501:HOH:O	2.13	0.64
1:A:256:ILE:HD11	1:A:259:LYS:CG	2.28	0.64
1:A:304:LYS:HD2	2:B:59:MET:HE1	1.80	0.64
1:C:208:ARG:NH1	4:C:432:HOH:O	2.05	0.63
1:C:276:THR:CG2	1:C:278:CYS:O	2.47	0.63
1:C:31:ASP:OD2	1:C:35:LYS:NZ	2.28	0.63
1:C:151:ILE:HG23	1:C:190:LEU:O	1.98	0.62
1:E:212:LYS:O	1:E:216:ARG:NH2	2.28	0.62
1:C:50:LEU:HD13	1:C:73:VAL:HG11	1.80	0.62
1:E:8:HIS:HB2	2:F:21:TRP:HA	1.82	0.62
1:E:196:THR:HB	1:E:245:GLY:HA3	1.81	0.62
1:E:257:VAL:HA	1:E:259:LYS:HZ1	1.65	0.62
1:C:5:ILE:HG13	2:D:119:TYR:HA	1.81	0.62
2:D:13:GLY:O	4:D:304:HOH:O	2.16	0.61
1:E:171:ASP:HB2	1:E:256:ILE:HG12	1.82	0.61
1:C:103:HIS:O	1:C:106:SER:OG	2.19	0.61
2:F:42:GLN:O	2:F:45:ILE:HG13	2.01	0.61
2:F:135:ASN:HD21	2:F:137:CYS:HB2	1.66	0.61
1:C:258:LYS:HG2	1:C:259:LYS:N	2.14	0.61
2:D:59:MET:O	2:D:61:THR:N	2.34	0.61
1:A:27:THR:HG22	1:A:316:GLY:HA3	1.83	0.60
2:B:141:TYR:C	2:B:169:LYS:HE3	2.20	0.60
1:A:186:GLU:HA	1:A:189:LYS:HG2	1.83	0.60
2:B:103:GLU:OE1	2:B:106:ARG:NH1	2.33	0.60
1:E:76:TRP:N	1:E:109:ASN:O	2.31	0.60
2:B:128:ASP:OD1	2:B:159:TYR:OH	2.13	0.60
1:E:57:VAL:O	1:E:60:TRP:HB3	2.02	0.60
1:A:5:ILE:HG13	2:B:119:TYR:HA	1.84	0.60
1:A:216:ARG:HD3	1:A:225:ARG:HD3	1.83	0.60
1:A:152:LYS:HE2	1:A:189:LYS:O	2.01	0.60
2:D:128:ASP:OD1	2:D:159:TYR:OH	2.18	0.59
1:C:106:SER:HA	1:C:262:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:HE3	1:A:301:GLU:HB2	1.84	0.59
1:E:60:TRP:HZ3	1:E:105:LEU:HD13	1.68	0.59
1:C:16:VAL:HG11	1:C:314:ALA:HB2	1.84	0.59
2:F:25:HIS:O	4:F:203:HOH:O	2.15	0.59
2:B:59:MET:O	2:B:61:THR:N	2.36	0.59
1:E:213:ILE:N	4:E:502:HOH:O	2.36	0.58
1:C:222:GLN:NE2	4:C:452:HOH:O	2.36	0.58
1:C:106:SER:HB2	4:C:411:HOH:O	2.02	0.58
1:C:0:GLY:N	4:C:444:HOH:O	2.35	0.58
1:A:285:ILE:HD11	1:A:287:SER:OG	2.04	0.58
1:E:306:VAL:HG13	1:E:308:SER:H	1.67	0.58
1:C:152:LYS:HE2	1:C:189:LYS:O	2.03	0.58
2:D:67:GLY:O	2:D:68:ARG:HB2	2.04	0.58
1:E:70:PHE:O	1:E:71:ILE:C	2.39	0.58
2:D:126:LEU:HD13	2:D:130:ALA:HB3	1.86	0.57
2:B:126:LEU:HD13	2:B:130:ALA:HB3	1.87	0.57
2:D:62:GLN:OE1	2:D:62:GLN:N	2.38	0.57
1:E:152:LYS:HE2	1:E:189:LYS:O	2.04	0.57
1:E:47:VAL:O	1:E:77:SER:OG	2.20	0.57
1:E:38:ASN:N	1:E:38:ASN:OD1	2.37	0.57
2:B:67:GLY:O	2:B:68:ARG:HB2	2.05	0.57
1:C:107:ARG:NH1	4:C:402:HOH:O	2.38	0.56
2:F:62:GLN:OE1	2:F:62:GLN:N	2.39	0.56
1:A:19:ILE:CD1	1:A:20:MET:HG3	2.34	0.56
1:C:33:LEU:O	1:C:35:LYS:NZ	2.38	0.56
1:E:21:GLU:OE2	1:E:318:ARG:NH2	2.39	0.56
1:A:216:ARG:HD3	1:A:225:ARG:CD	2.35	0.56
1:C:246:ASN:N	1:C:246:ASN:OD1	2.38	0.55
1:E:246:ASN:N	1:E:246:ASN:OD1	2.39	0.55
2:F:164:GLU:HA	2:F:167:ARG:HG2	1.89	0.55
1:C:209:LEU:HA	4:C:403:HOH:O	2.05	0.55
2:F:151:SER:OG	2:F:157:TYR:HA	2.06	0.55
2:D:169:LYS:HA	2:D:172:GLU:HG3	1.89	0.54
2:D:169:LYS:HB3	4:D:306:HOH:O	2.05	0.54
2:F:30:GLN:NE2	2:F:146:ASN:OD1	2.40	0.54
1:A:193:ASN:ND2	1:A:244:ASN:O	2.37	0.54
1:C:73:VAL:HG12	1:C:74:PRO:O	2.07	0.54
1:A:246:ASN:OD1	1:A:246:ASN:N	2.40	0.54
1:C:108:ILE:HD13	1:C:256:ILE:HD12	1.89	0.54
2:F:52:VAL:O	2:F:55:ILE:HG22	2.08	0.54
1:E:119:LYS:N	4:E:505:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:MET:O	2:F:61:THR:N	2.40	0.54
1:E:171:ASP:O	1:E:256:ILE:HG13	2.08	0.54
2:F:132:GLU:HG2	2:F:138:PHE:CE1	2.43	0.53
1:E:116:ILE:HD11	1:E:164:TYR:CD2	2.43	0.53
1:A:107:ARG:HA	1:A:260:GLY:O	2.09	0.53
2:D:151:SER:OG	2:D:157:TYR:HA	2.09	0.53
2:D:38:LYS:HG3	2:D:39:GLU:N	2.23	0.53
1:C:53:ARG:HG3	1:C:54:ASP:H	1.74	0.53
1:A:27:THR:HG22	1:A:317:LEU:H	1.73	0.52
1:E:285:ILE:HD11	1:E:287:SER:OG	2.08	0.52
1:A:191:TYR:O	1:A:192:GLN:HB2	2.08	0.52
2:F:51:LYS:HE2	2:F:103:GLU:CG	2.32	0.52
1:E:78:TYR:HA	1:E:262:SER:HB3	1.91	0.52
2:D:167:ARG:NE	4:D:326:HOH:O	2.34	0.52
2:F:135:ASN:ND2	2:F:137:CYS:HB2	2.24	0.52
1:A:44:LEU:HD11	1:A:299:ILE:HD11	1.91	0.52
1:E:307:LYS:HD2	2:F:89:LEU:HD21	1.92	0.52
2:F:165:GLU:O	2:F:169:LYS:HG2	2.10	0.52
1:E:110:HIS:HB3	1:E:257:VAL:O	2.10	0.52
1:E:30:GLN:OE1	2:F:52:VAL:HG11	2.10	0.51
1:C:62:LEU:O	1:C:144:PHE:HB3	2.10	0.51
1:A:191:TYR:O	1:A:192:GLN:CB	2.58	0.51
2:B:51:LYS:HE2	2:B:106:ARG:HH12	1.75	0.51
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.20	0.51
2:F:172:GLU:OE1	2:F:172:GLU:N	2.42	0.51
2:F:109:ASP:OD1	2:F:112:ASP:HB2	2.11	0.51
1:C:138:GLN:NE2	4:C:438:HOH:O	2.25	0.51
2:B:75:ARG:NH1	2:B:78:GLU:OE2	2.42	0.51
2:F:24:TYR:CD1	2:F:153:ARG:HD3	2.46	0.51
1:E:53:ARG:HG3	1:E:54:ASP:H	1.76	0.51
1:C:308:SER:HB3	2:D:97:GLU:OE2	2.11	0.50
2:B:23:GLY:HA3	2:B:36:ALA:HA	1.93	0.50
1:C:263:ALA:HB3	1:C:299:ILE:HD12	1.92	0.50
2:F:121:LYS:O	2:F:125:GLN:OE1	2.29	0.50
1:E:277:LYS:HG2	1:E:301:GLU:HB3	1.93	0.50
1:A:108:ILE:HG22	1:A:109:ASN:N	2.26	0.50
1:C:306:VAL:CG2	2:D:93:THR:HA	2.42	0.50
1:C:123:SER:O	1:C:153:LYS:NZ	2.39	0.50
2:D:59:MET:C	2:D:61:THR:N	2.64	0.50
1:C:280:THR:HG23	1:C:282:ILE:H	1.75	0.50
1:E:27:THR:O	1:E:28:HIS:ND1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:HG23	2:B:105:GLU:HB2	1.95	0.49
2:F:59:MET:C	2:F:61:THR:H	2.15	0.49
1:A:107:ARG:CD	1:A:260:GLY:O	2.52	0.49
1:E:178:ILE:HG13	1:E:209:LEU:HD23	1.93	0.49
2:F:63:PHE:N	2:F:63:PHE:CD2	2.80	0.49
1:E:109:ASN:OD1	1:E:258:LYS:HG2	2.13	0.49
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.95	0.49
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.95	0.48
1:E:290:PRO:HD3	2:F:56:ILE:HG12	1.95	0.48
2:F:68:ARG:HG3	2:F:69:GLU:H	1.79	0.48
1:A:123:SER:O	1:A:153:LYS:NZ	2.40	0.48
2:B:128:ASP:O	2:B:141:TYR:CD2	2.67	0.47
2:D:89:LEU:HD23	2:D:89:LEU:C	2.35	0.47
2:D:165:GLU:O	2:D:169:LYS:HG2	2.14	0.47
1:E:90:CYS:HB2	1:E:135:CYS:HA	1.96	0.47
2:F:24:TYR:OH	2:F:118:LEU:HD11	2.14	0.47
2:B:39:GLU:O	2:B:43:LYS:HD3	2.15	0.47
1:E:257:VAL:HA	1:E:258:LYS:HA	1.69	0.47
2:B:59:MET:C	2:B:61:THR:H	2.17	0.47
1:C:257:VAL:HA	1:C:258:LYS:HA	1.70	0.47
1:A:299:ILE:HG13	1:A:299:ILE:O	2.15	0.47
1:A:27:THR:HG21	1:A:317:LEU:HD12	1.97	0.46
1:C:126:GLU:OE1	4:C:427:HOH:O	2.20	0.46
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.27	0.46
1:A:52:LEU:HA	1:A:70:PHE:CZ	2.50	0.46
2:D:68:ARG:HG2	2:D:70:PHE:CZ	2.51	0.46
1:A:298:THR:HG22	1:A:302:CYS:SG	2.55	0.46
1:C:147:VAL:HG13	1:C:248:ILE:HG22	1.98	0.46
1:A:62:LEU:O	1:A:144:PHE:HB3	2.16	0.46
2:B:82:LYS:NZ	2:B:86:ASP:OD2	2.45	0.46
1:C:307:LYS:CE	2:D:89:LEU:HD21	2.39	0.46
1:C:110:HIS:HB3	1:C:257:VAL:O	2.16	0.46
2:B:142:HIS:HA	2:B:169:LYS:NZ	2.30	0.46
2:B:169:LYS:HB3	2:B:169:LYS:HE2	1.45	0.46
2:F:17:MET:HE1	2:F:34:TYR:HB3	1.98	0.46
2:B:128:ASP:O	2:B:141:TYR:HD2	1.97	0.46
2:B:150:GLU:OE1	2:B:153:ARG:NH1	2.49	0.46
2:D:24:TYR:CD1	2:D:153:ARG:HD3	2.52	0.45
1:E:316:GLY:C	2:F:111:HIS:HE1	2.19	0.45
1:E:109:ASN:CG	1:E:258:LYS:HG2	2.36	0.45
1:A:147:VAL:HG13	1:A:248:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:O	1:C:71:ILE:HG13	2.17	0.45
1:C:10:ASN:OD1	1:C:12:SER:HB3	2.17	0.45
1:C:27:THR:O	1:C:28:HIS:ND1	2.49	0.45
1:A:115:GLN:NE2	4:A:533:HOH:O	2.37	0.45
1:E:153:LYS:O	1:E:156:THR:OG1	2.29	0.45
1:A:137:TYR:HB2	1:A:142:SER:OG	2.17	0.45
2:D:128:ASP:O	2:D:141:TYR:HD2	2.00	0.45
2:B:24:TYR:CD1	2:B:153:ARG:HD3	2.53	0.44
1:A:116:ILE:HD11	1:A:164:TYR:CZ	2.52	0.44
1:A:130:GLY:CA	1:A:149:TRP:HB3	2.47	0.44
1:A:10:ASN:OD1	1:A:12:SER:HB3	2.16	0.44
2:F:126:LEU:O	2:F:127:ARG:C	2.55	0.44
1:E:109:ASN:ND2	1:E:258:LYS:HG2	2.32	0.44
2:B:55:ILE:HG12	2:B:99:LEU:HD21	1.99	0.44
1:C:280:THR:HG22	1:C:283:GLY:O	2.18	0.44
1:C:255:LYS:HE3	1:C:255:LYS:HB3	1.64	0.44
1:E:207:GLN:CD	1:E:209:LEU:HD11	2.38	0.44
1:E:258:LYS:C	1:E:259:LYS:HE3	2.37	0.44
1:E:62:LEU:O	1:E:144:PHE:HB3	2.18	0.44
2:D:170:ARG:O	2:D:173:ILE:HG22	2.17	0.44
1:E:116:ILE:HG23	1:E:117:ILE:HG12	1.99	0.44
2:F:67:GLY:O	2:F:68:ARG:HB2	2.18	0.44
1:E:112:GLU:HB3	1:E:255:LYS:HG2	1.99	0.44
1:C:47:VAL:HG13	1:C:77:SER:HB3	1.98	0.44
1:A:107:ARG:HD2	1:A:107:ARG:HA	1.61	0.43
1:C:166:ASN:O	1:C:235:PRO:O	2.36	0.43
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.82	0.43
1:A:307:LYS:CE	2:B:89:LEU:HD21	2.42	0.43
1:A:304:LYS:HE2	2:B:92:TRP:CG	2.53	0.43
2:D:75:ARG:NH1	2:D:78:GLU:OE2	2.47	0.43
2:F:147:GLU:OE1	2:F:147:GLU:HA	2.18	0.43
1:C:257:VAL:HG13	1:C:257:VAL:O	2.18	0.43
1:A:108:ILE:CG2	1:A:109:ASN:N	2.82	0.43
1:A:281:PRO:HD3	1:A:297:LEU:O	2.18	0.43
1:A:161:LYS:HG3	1:A:242:GLU:HG3	2.01	0.43
1:A:116:ILE:HD11	1:A:164:TYR:CE2	2.54	0.43
1:E:112:GLU:HB3	1:E:255:LYS:CG	2.48	0.43
1:A:8:HIS:HB3	1:A:317:LEU:HD13	2.00	0.43
1:E:68:ASP:O	1:E:71:ILE:HG12	2.19	0.43
1:A:114:ILE:HD11	1:A:255:LYS:HE3	1.96	0.43
2:B:89:LEU:C	2:B:89:LEU:HD23	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:TYR:N	2:F:160:PRO:HD2	2.33	0.43
1:E:166:ASN:O	1:E:235:PRO:O	2.36	0.43
1:C:137:TYR:HB2	1:C:142:SER:HB2	2.00	0.43
1:E:306:VAL:CG2	2:F:93:THR:HA	2.49	0.43
1:A:110:HIS:HB3	1:A:257:VAL:O	2.19	0.43
1:E:181:SER:HB2	1:E:186:GLU:OE2	2.19	0.43
1:E:257:VAL:HG13	1:E:257:VAL:O	2.19	0.42
1:A:234:LYS:NZ	4:A:508:HOH:O	2.08	0.42
2:B:167:ARG:HG3	2:B:171:GLU:OE1	2.19	0.42
1:A:166:ASN:O	1:A:235:PRO:O	2.36	0.42
1:E:302:CYS:HA	1:E:303:PRO:HD2	1.90	0.42
1:E:171:ASP:O	1:E:256:ILE:CG1	2.68	0.42
2:F:160:PRO:HA	2:F:163:SER:HB3	2.02	0.42
1:E:107:ARG:HA	1:E:260:GLY:O	2.18	0.42
2:B:159:TYR:N	2:B:160:PRO:HD2	2.34	0.42
1:C:107:ARG:HD3	4:C:402:HOH:O	2.18	0.42
2:B:146:ASN:ND2	4:B:312:HOH:O	2.30	0.42
1:C:77:SER:OG	1:C:78:TYR:HD2	2.02	0.42
2:F:133:LEU:HD11	2:F:139:GLU:HB2	2.02	0.42
1:C:287:SER:OG	1:C:288:SER:N	2.52	0.42
1:E:8:HIS:CD2	2:F:20:GLY:O	2.73	0.41
1:A:27:THR:CG2	1:A:317:LEU:H	2.32	0.41
1:E:45:ASP:O	1:E:47:VAL:HG13	2.20	0.41
1:C:306:VAL:HG13	1:C:308:SER:H	1.83	0.41
2:F:149:MET:O	2:F:152:VAL:HG22	2.20	0.41
1:C:51:ILE:HA	1:C:80:VAL:HG13	2.02	0.41
1:A:257:VAL:O	1:A:257:VAL:HG13	2.20	0.41
1:E:218:LYS:HE3	1:E:221:GLY:HA2	2.02	0.41
1:A:53:ARG:HG3	1:A:54:ASP:H	1.85	0.41
1:E:256:ILE:HD13	1:E:259:LYS:HD3	2.03	0.41
1:E:316:GLY:O	2:F:111:HIS:HE1	2.04	0.41
1:E:137:TYR:HB2	1:E:142:SER:CB	2.51	0.41
1:E:259:LYS:N	1:E:259:LYS:HE3	2.36	0.41
1:E:274:CYS:SG	1:E:275:ASN:N	2.93	0.41
1:C:302:CYS:HA	1:C:303:PRO:HD2	1.84	0.41
1:C:47:VAL:CG1	1:C:77:SER:HB3	2.51	0.41
1:C:137:TYR:HB2	1:C:142:SER:CB	2.50	0.41
1:C:13:THR:OG1	4:C:439:HOH:O	2.22	0.41
1:E:121:SER:CB	1:E:162:ARG:HH22	2.34	0.41
1:E:160:ILE:HG12	1:E:243:SER:O	2.21	0.41
1:E:318:ARG:HE	2:F:108:LEU:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HG13	1:C:80:VAL:CG1	2.51	0.40
1:E:51:ILE:HA	1:E:80:VAL:HG13	2.03	0.40
1:C:52:LEU:HA	1:C:70:PHE:CZ	2.57	0.40
2:B:94:TYR:CZ	2:B:98:LEU:HD12	2.57	0.40
1:E:137:TYR:HB2	1:E:142:SER:HB2	2.03	0.40
2:D:71:ASN:OD1	2:D:74:GLU:HG3	2.22	0.40
1:E:106:SER:HB2	1:E:263:ALA:HA	2.04	0.40
2:B:99:LEU:O	2:B:103:GLU:HB2	2.22	0.40
1:C:32:ILE:O	1:C:289:MET:HB3	2.22	0.40
1:C:155:ASN:O	1:C:192:GLN:HG3	2.20	0.40
2:F:164:GLU:HB3	2:F:167:ARG:NH2	2.37	0.40
1:E:317:LEU:HG	2:F:111:HIS:CE1	2.57	0.40
1:A:51:ILE:HA	1:A:80:VAL:HG13	2.04	0.40
1:C:130:GLY:CA	1:C:149:TRP:HB3	2.51	0.40
2:F:151:SER:OG	2:F:156:THR:O	2.38	0.40
2:B:51:LYS:HE2	2:B:103:GLU:HG3	2.03	0.40
2:D:126:LEU:O	2:D:127:ARG:C	2.60	0.40
2:D:149:MET:O	2:D:152:VAL:HG22	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ARG:NH1	2:D:79:ASN:OD1[2_655]	2.18	0.02

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	321/329 (98%)	290 (90%)	27 (8%)	4 (1%)	16 39
1	C	320/329 (97%)	289 (90%)	29 (9%)	2 (1%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	320/329 (97%)	294 (92%)	25 (8%)	1 (0%)	46 75
2	B	162/174 (93%)	153 (94%)	6 (4%)	3 (2%)	10 25
2	D	162/174 (93%)	153 (94%)	6 (4%)	3 (2%)	10 25
2	F	162/174 (93%)	150 (93%)	9 (6%)	3 (2%)	10 25
All	All	1447/1509 (96%)	1329 (92%)	102 (7%)	16 (1%)	17 42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	68	ARG
2	D	68	ARG
2	D	127	ARG
2	F	68	ARG
2	F	127	ARG
2	B	127	ARG
2	D	60	ASN
2	F	60	ASN
1	A	192	GLN
1	C	166	ASN
1	E	235	PRO
1	A	105	LEU
1	A	235	PRO
1	C	235	PRO
1	A	166	ASN

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	288/293 (98%)	261 (91%)	27 (9%)	11 25
1	C	287/293 (98%)	264 (92%)	23 (8%)	15 33
1	E	287/293 (98%)	261 (91%)	26 (9%)	12 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	144/149 (97%)	135 (94%)	9 (6%)	22 48
2	D	144/149 (97%)	134 (93%)	10 (7%)	19 43
2	F	144/149 (97%)	137 (95%)	7 (5%)	31 61
All	All	1294/1326 (98%)	1192 (92%)	102 (8%)	15 34

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	26	VAL
1	A	27	THR
1	A	52	LEU
1	A	80	VAL
1	A	91	TYR
1	A	107	ARG
1	A	109	ASN
1	A	133	SER
1	A	137	TYR
1	A	147	VAL
1	A	188	THR
1	A	192	GLN
1	A	193	ASN
1	A	204	THR
1	A	207	GLN
1	A	208	ARG
1	A	212	LYS
1	A	223	SER
1	A	225	ARG
1	A	235	PRO
1	A	246	ASN
1	A	256	ILE
1	A	274	CYS
1	A	280	THR
1	A	299	ILE
1	A	306	VAL
2	B	10	ILE
2	B	40	SER
2	B	66	VAL
2	B	113	SER
2	B	127	ARG
2	B	133	LEU

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Mol	Chain	Res	Type
2	B	149	MET
2	B	167	ARG
2	B	169	LYS
1	C	26	VAL
1	C	27	THR
1	C	47	VAL
1	C	80	VAL
1	C	91	TYR
1	C	105	LEU
1	C	133	SER
1	C	142	SER
1	C	147	VAL
1	C	188	THR
1	C	193	ASN
1	C	204	THR
1	C	208	ARG
1	C	212	LYS
1	C	235	PRO
1	C	246	ASN
1	C	255	LYS
1	C	262	SER
1	C	274	CYS
1	C	276	THR
1	C	280	THR
1	C	298	THR
1	C	306	VAL
2	D	28	ASN
2	D	49	THR
2	D	61	THR
2	D	66	VAL
2	D	68	ARG
2	D	90	ASP
2	D	106	ARG
2	D	113	SER
2	D	127	ARG
2	D	149	MET
1	E	10	ASN
1	E	16	VAL
1	E	26	VAL
1	E	38	ASN
1	E	44	LEU
1	E	47	VAL

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Mol	Chain	Res	Type
1	E	51	ILE
1	E	70	PHE
1	E	80	VAL
1	E	91	TYR
1	E	106	SER
1	E	133	SER
1	E	142	SER
1	E	178	ILE
1	E	188	THR
1	E	193	ASN
1	E	204	THR
1	E	208	ARG
1	E	246	ASN
1	E	259	LYS
1	E	262	SER
1	E	270	GLU
1	E	274	CYS
1	E	280	THR
1	E	298	THR
1	E	306	VAL
2	F	43	LYS
2	F	49	THR
2	F	61	THR
2	F	63	PHE
2	F	113	SER
2	F	149	MET
2	F	156	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	295	HIS
2	B	142	HIS
1	C	30	GLN
1	C	182	ASN
1	C	295	HIS
2	D	28	ASN
2	D	146	ASN
1	E	10	ASN
1	E	286	ASN
2	F	111	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

4 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	401	1	14,14,15	0.95	1 (7%)	15,19,21	1.45	2 (13%)
3	NAG	B	201	2	14,14,15	0.44	0	15,19,21	0.73	0
3	NAG	D	201	2	14,14,15	0.41	0	15,19,21	0.80	1 (6%)
3	NAG	E	401	1	14,14,15	0.79	1 (7%)	15,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	201	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	201	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	401	1	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	NAG	O5-C1	-2.10	1.40	1.43
3	A	401	NAG	C1-C2	2.60	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	NAG	O6-C6-C5	-2.76	102.23	111.33
3	D	201	NAG	O5-C5-C6	2.03	111.75	107.35
3	A	401	NAG	C4-C3-C2	2.61	115.29	111.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	401	NAG	C1
3	D	201	NAG	C1
3	B	201	NAG	C1
3	A	401	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	323/329 (98%)	-0.16	6 (1%) 70 70	29, 70, 109, 129	0
1	C	322/329 (97%)	-0.04	3 (0%) 85 86	36, 67, 114, 144	0
1	E	322/329 (97%)	0.46	22 (6%) 20 19	54, 107, 165, 188	0
2	B	164/174 (94%)	0.09	4 (2%) 62 62	39, 87, 123, 166	0
2	D	164/174 (94%)	-0.01	2 (1%) 81 81	25, 72, 117, 144	0
2	F	164/174 (94%)	1.35	48 (29%) 1 0	61, 142, 199, 220	0
All	All	1459/1509 (96%)	0.22	85 (5%) 26 25	25, 83, 165, 220	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	157	TYR	10.4
2	F	130	ALA	9.5
2	F	35	ALA	8.9
2	F	129	ASN	8.6
2	F	33	GLY	6.5
1	C	217	SER	5.9
1	E	286	ASN	5.5
1	E	220	ASN	5.4
2	F	26	HIS	5.4
2	F	19	ASP	4.9
1	C	321	PRO	4.8
1	E	219	VAL	4.7
2	F	144	CYS	4.7
2	F	133	LEU	4.7
2	F	34	TYR	4.6
2	F	24	TYR	4.3
2	F	21	TRP	4.1
1	E	260	GLY	4.0
2	F	14	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	138	PHE	3.8
2	F	32	SER	3.8
2	F	109	ASP	3.8
1	E	108	ILE	3.8
2	F	29	GLU	3.7
1	A	309	ASN	3.7
2	F	140	PHE	3.6
2	F	131	LYS	3.6
2	F	27	SER	3.6
2	F	36	ALA	3.6
2	F	152	VAL	3.5
1	A	308	SER	3.5
1	E	271	TYR	3.4
2	F	128	ASP	3.4
2	F	145	ASP	3.4
1	E	217	SER	3.4
2	F	112	ASP	3.2
1	E	135	CYS	3.2
1	E	6	GLY	3.1
1	E	3	ILE	3.1
2	D	157	TYR	3.1
2	F	141	TYR	3.1
1	A	291	PHE	3.0
1	E	106	SER	3.0
1	E	91	TYR	3.0
2	F	155	GLY	3.0
1	C	219	VAL	2.9
2	F	25	HIS	2.9
2	F	118	LEU	2.9
1	E	40	LYS	2.9
2	F	160	PRO	2.8
1	E	110	HIS	2.7
1	A	305	TYR	2.7
1	A	321	PRO	2.7
2	F	158	ASP	2.7
1	E	218	LYS	2.6
2	F	108	LEU	2.6
1	E	41	LEU	2.5
2	F	10	ILE	2.5
2	F	149	MET	2.5
1	A	297	LEU	2.5
2	F	148	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	115	VAL	2.4
2	F	31	GLY	2.3
2	B	20	GLY	2.3
2	F	162	TYR	2.3
1	E	70	PHE	2.3
2	F	123	ARG	2.3
1	E	130	GLY	2.3
2	F	22	TYR	2.2
1	E	262	SER	2.2
2	F	23	GLY	2.2
2	F	139	GLU	2.2
2	B	11	GLU	2.2
2	F	147	GLU	2.2
2	F	60	ASN	2.1
1	E	261	ASP	2.1
1	E	201	GLY	2.1
2	F	30	GLN	2.1
2	B	160	PRO	2.1
2	D	160	PRO	2.1
2	B	106	ARG	2.0
1	E	1	ASP	2.0
2	F	159	TYR	2.0
2	F	114	ASN	2.0
2	F	126	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	401	14/15	0.93	0.16	-0.45	82,93,98,109	0
3	NAG	E	401	14/15	0.85	0.16	-1.01	78,101,112,117	0
3	NAG	B	201	14/15	0.73	0.46	-	132,144,154,167	0
3	NAG	D	201	14/15	0.85	0.56	-	109,140,147,151	0

6.5 Other polymers (i)

There are no such residues in this entry.