Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 09:22 am GMT

PDB ID	:	2VUS
Title	:	Crystal structure of unliganded NmrA-AreA zinc finger complex
Authors	:	Kotaka, M.; Johnson, C.; Lamb, H.K.; Hawkins, A.R.; Ren, J.; Stammers, D.K.
Deposited on	:	2008-05-30
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

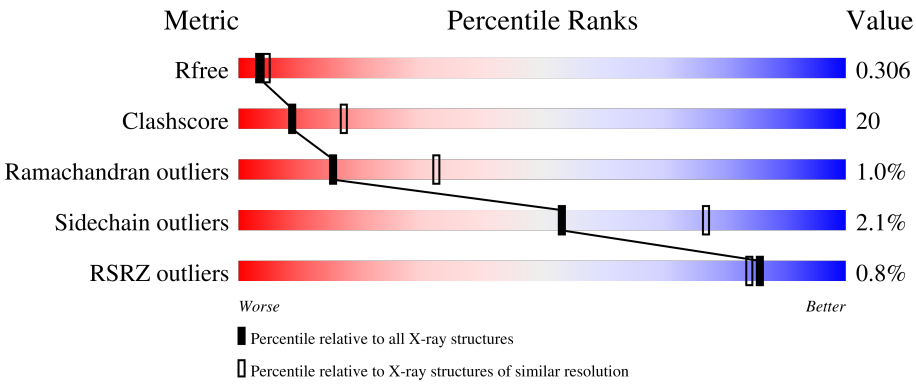
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	352	49% 40% • 10%
1	B	352	54% 35% • 10%
1	C	352	54% 35% • 10%
1	D	352	49% 40% • 10%
1	E	352	61% 28% • 10%

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Mol	Chain	Length	Quality of chain
1	F	352	% 59% 31% • 10%
1	G	352	59% 30% • 10%
1	H	352	59% 30% • 10%
2	I	43	7% 63% 35% •
2	J	43	2% 56% 40% • •
2	K	43	5% 51% 40% 5% 5%
2	L	43	56% 42% •
2	M	43	9% 67% 30% •
2	N	43	5% 63% 35% •
2	O	43	7% 63% 30% • 5%
2	P	43	9% 63% 33% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24506 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 NITROGEN METABOLITE REPRESSION REGULATOR NMRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2530	1637	428	457	8	0	0	0
1	B	318	2530	1637	428	457	8	0	0	0
1	C	318	2530	1637	428	457	8	0	0	0
1	D	318	2530	1637	428	457	8	0	0	0
1	E	318	2530	1637	428	457	8	0	0	0
1	F	318	2530	1637	428	457	8	0	0	0
1	G	318	2530	1637	428	457	8	0	0	0
1	H	318	2530	1637	428	457	8	0	0	0

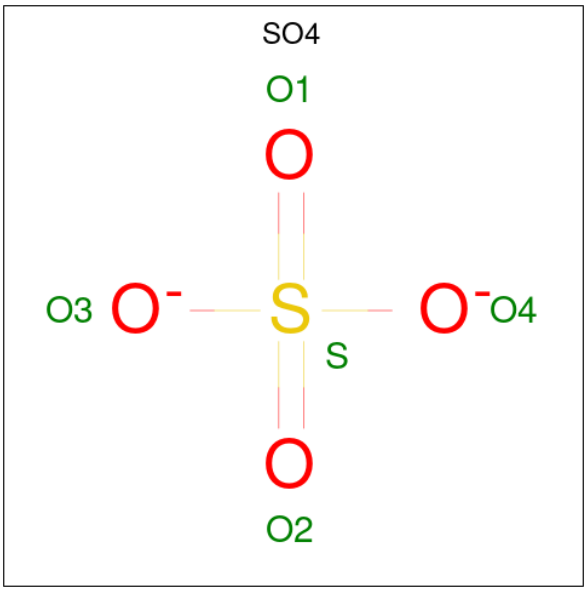
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ARG	LEU	conflict	UNP O59919
B	238	ARG	LEU	conflict	UNP O59919
C	238	ARG	LEU	conflict	UNP O59919
D	238	ARG	LEU	conflict	UNP O59919
E	238	ARG	LEU	conflict	UNP O59919
F	238	ARG	LEU	conflict	UNP O59919
G	238	ARG	LEU	conflict	UNP O59919
H	238	ARG	LEU	conflict	UNP O59919

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN AREA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	42	326	206	60	56	4	0	0	0
2	J	42	326	206	60	56	4	0	0	0
2	K	41	318	200	59	55	4	0	0	0
2	L	42	326	206	60	56	4	0	0	0
2	M	43	333	211	61	57	4	0	0	0
2	N	42	326	206	60	56	4	0	0	0
2	O	41	318	200	59	55	4	0	0	0
2	P	42	326	206	60	56	4	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	E	1	5	4	1	0	0
3	F	1	5	4	1	0	0
3	G	1	5	4	1	0	0
3	H	1	5	4	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0
4	F	1	1	1	0	0
4	G	2	2	2	0	0
4	H	1	1	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	I	1	1	1	0	0
5	J	1	1	1	0	0
5	K	1	1	1	0	0
5	L	1	1	1	0	0
5	M	1	1	1	0	0
5	N	1	1	1	0	0
5	O	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	P	1	1	1	0	0

- Molecule 6 is water.

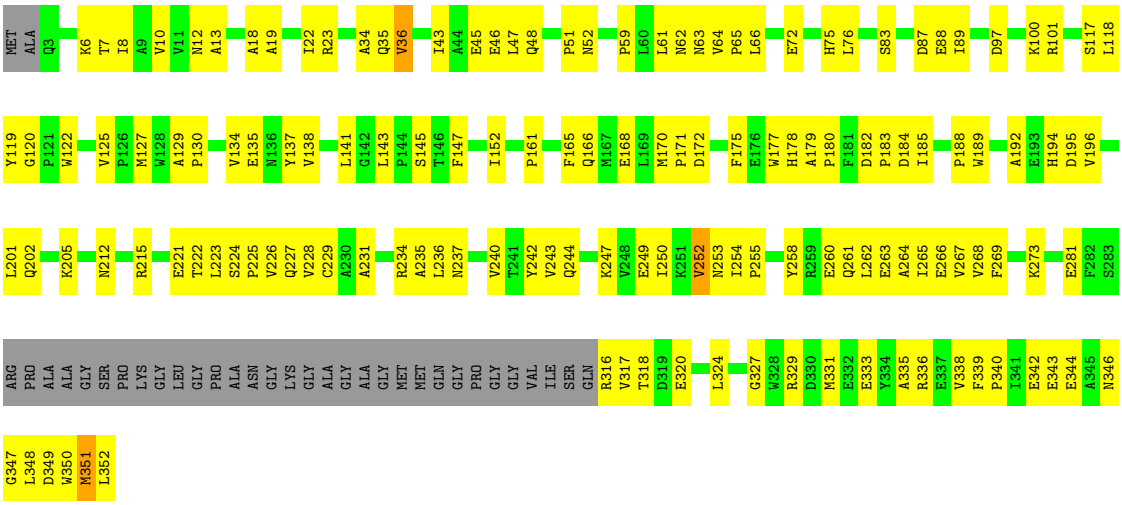
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	148	148	148	0	0
			Total	O		
6	B	181	181	181	0	0
			Total	O		
6	C	192	192	192	0	0
			Total	O		
6	D	184	184	184	0	0
			Total	O		
6	E	207	207	207	0	0
			Total	O		
6	F	170	170	170	0	0
			Total	O		
6	G	212	212	212	0	0
			Total	O		
6	H	177	177	177	0	0
			Total	O		
6	I	26	26	26	0	0
			Total	O		
6	J	17	17	17	0	0
			Total	O		
6	K	20	20	20	0	0
			Total	O		
6	L	16	16	16	0	0
			Total	O		
6	M	17	17	17	0	0
			Total	O		
6	N	17	17	17	0	0
			Total	O		
6	O	17	17	17	0	0
			Total	O		
6	P	11	11	11	0	0

3 Residue-property plots (i)

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

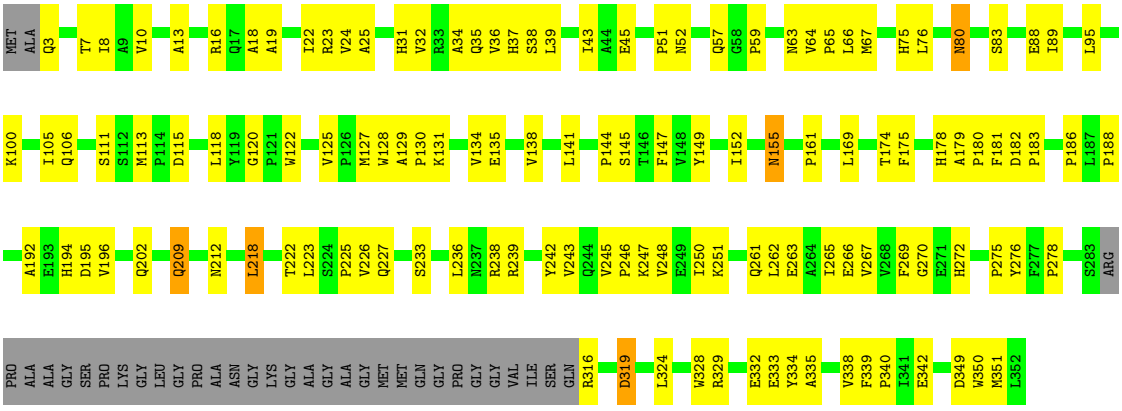
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain A: 49% 40% • 10%



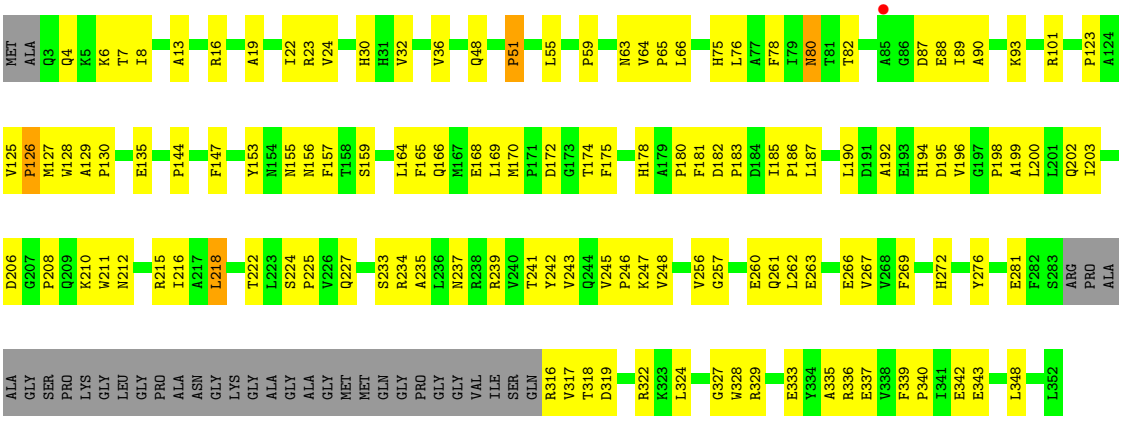
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain B: 54% 35% • 10%



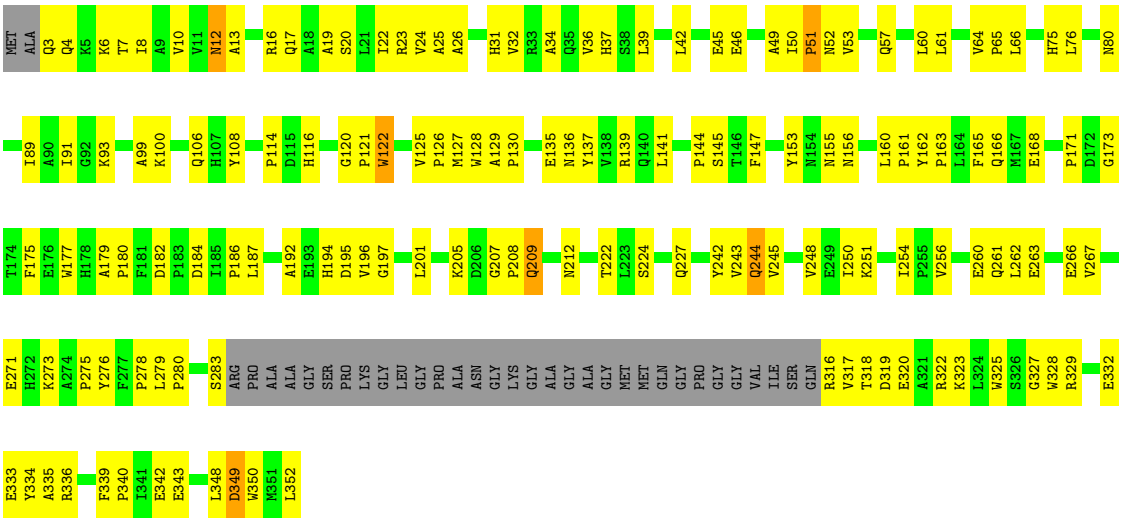
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain C: 54% 35% • 10%



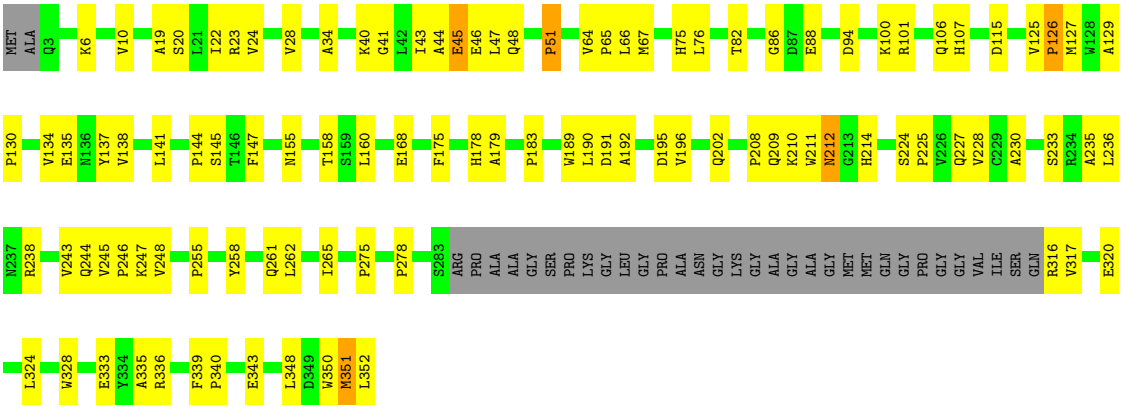
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain D: 49% 40% • 10%



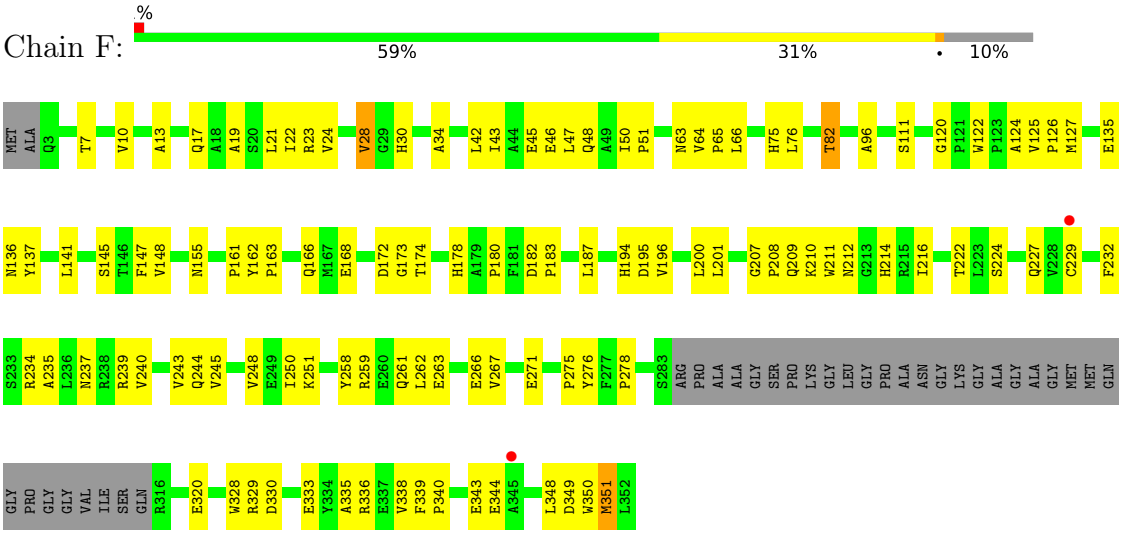
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain E: 61% 28% • 10%



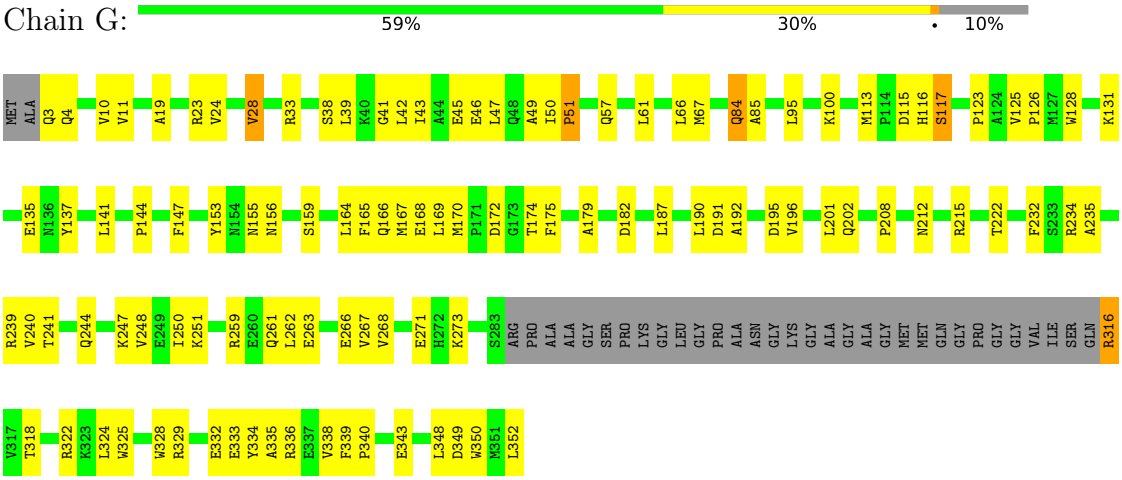
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain F:



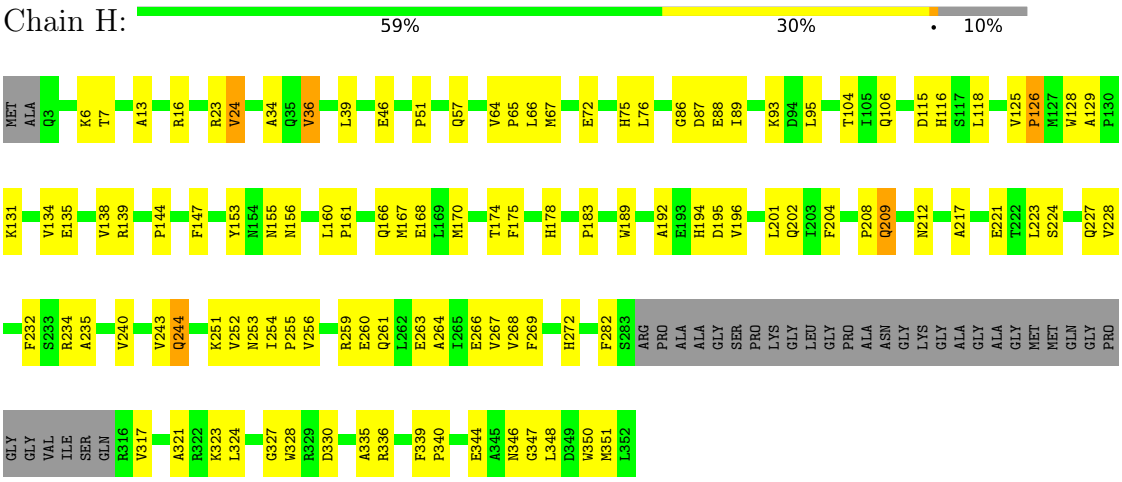
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain G:



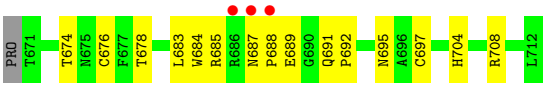
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain H:



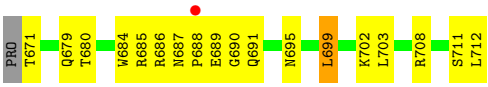
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain I:



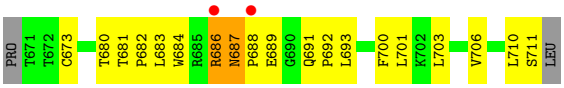
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain J:



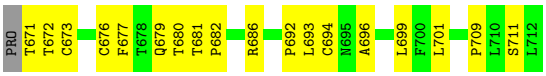
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain K:



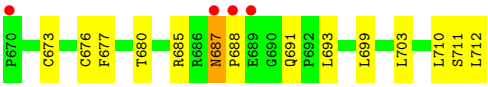
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain L:



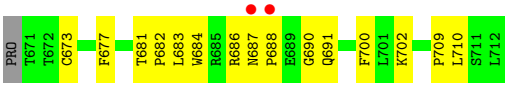
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain M:



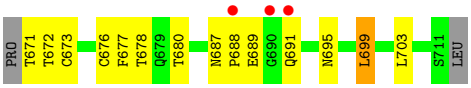
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain N:



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

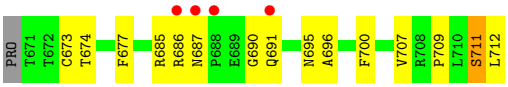
Chain O:



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain P:

9%
63%
33%


PRO
T671
T672
C673
T674
F677
R685
R686
N687
P688
E689
G690
Q691
N695
A696
F700
V707
R708
P709
L710
S711
L712

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	228.79Å 228.79Å 222.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 2.60 29.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.97-2.60) 98.8 (29.97-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.306 0.243 , 0.306	Depositor DCC
R_{free} test set	6691 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 18.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.387 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24506	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/2606	0.64	0/3557
1	B	0.38	0/2606	0.67	0/3557
1	C	0.39	0/2606	0.64	0/3557
1	D	0.39	0/2606	0.65	0/3557
1	E	0.39	0/2606	0.66	0/3557
1	F	0.38	0/2606	0.63	0/3557
1	G	0.40	0/2606	0.66	1/3557 (0.0%)
1	H	0.38	0/2606	0.64	0/3557
2	I	0.39	0/334	0.61	0/456
2	J	0.38	0/334	0.65	0/456
2	K	0.38	0/326	0.66	0/445
2	L	0.35	0/334	0.64	0/456
2	M	0.37	0/342	0.58	0/467
2	N	0.39	0/334	0.63	0/456
2	O	0.41	0/326	0.60	0/445
2	P	0.38	0/334	0.64	0/456
All	All	0.39	0/23512	0.65	1/32093 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	167	MET	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2530	0	2476	127	0
1	B	2530	0	2476	106	0
1	C	2530	0	2476	103	0
1	D	2530	0	2476	123	0
1	E	2530	0	2476	89	0
1	F	2530	0	2476	103	0
1	G	2530	0	2476	92	0
1	H	2530	0	2476	88	0
2	I	326	0	326	11	0
2	J	326	0	326	18	0
2	K	318	0	315	25	0
2	L	326	0	326	16	0
2	M	333	0	334	11	0
2	N	326	0	326	15	0
2	O	318	0	315	13	0
2	P	326	0	326	12	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1	0	0	0	0
6	A	148	0	0	11	0
6	B	181	0	0	17	0
6	C	192	0	0	13	0
6	D	184	0	0	18	0
6	E	207	0	0	10	0
6	F	170	0	0	9	0
6	G	212	0	0	18	0
6	H	177	0	0	8	0
6	I	26	0	0	0	0
6	J	17	0	0	3	0
6	K	20	0	0	0	0
6	L	16	0	0	3	0
6	M	17	0	0	0	0
6	N	17	0	0	3	0
6	O	17	0	0	0	0
6	P	11	0	0	0	0
All	All	24506	0	22402	924	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (924) 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)
2:J:687:ASN:HD21	2:J:691:GLN:HB2	1.14	1.06
1:G:352:LEU:OXT	6:G:2212:HOH:O	1.72	1.06
2:N:687:ASN:HD22	2:N:691:GLN:HB2	1.17	1.05
1:A:261:GLN:HE21	1:A:265:ILE:HD11	1.21	1.04
2:O:687:ASN:HD21	2:O:691:GLN:HB2	1.19	1.01
1:F:224:SER:H	1:F:227:GLN:NE2	1.60	0.98
1:E:235:ALA:HB1	1:E:336:ARG:HB2	1.41	0.98
1:F:224:SER:H	1:F:227:GLN:HE21	1.03	0.96
1:G:259:ARG:O	1:G:263:GLU:HG3	1.62	0.95
1:D:182:ASP:HB2	1:D:273:LYS:NZ	1.83	0.94
1:E:6:LYS:HE2	1:E:106:GLN:HE22	1.31	0.94
1:B:115:ASP:HB3	1:B:118:LEU:HD12	1.49	0.93
1:F:235:ALA:HB1	1:F:336:ARG:HB2	1.52	0.92
1:D:42:LEU:O	1:D:45:GLU:HG2	1.70	0.91
1:A:234:ARG:HG3	1:B:233:SER:HB3	1.50	0.91
1:D:182:ASP:HB2	1:D:273:LYS:HZ3	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:LEU:O	1:F:45:GLU:HG2	1.73	0.87
1:G:84:GLN:H	1:G:84:GLN:HE21	1.21	0.86
1:B:155:ASN:HD22	1:B:155:ASN:H	1.23	0.85
1:E:352:LEU:HD12	1:E:352:LEU:OXT	1.76	0.85
1:D:80:ASN:HB3	6:D:2063:HOH:O	1.76	0.85
2:L:672:THR:HG22	2:L:679:GLN:HG2	1.59	0.84
2:J:687:ASN:ND2	2:J:691:GLN:HB2	1.92	0.84
1:B:7:THR:H	1:B:75:HIS:HD2	1.21	0.83
2:O:687:ASN:ND2	2:O:691:GLN:HB2	1.92	0.83
1:H:7:THR:H	1:H:75:HIS:HD2	1.21	0.83
1:A:35:GLN:HG3	1:A:66:LEU:HD21	1.60	0.83
1:D:114:PRO:HB3	1:D:279:LEU:HD11	1.61	0.82
2:M:687:ASN:HB2	2:M:691:GLN:HB2	1.61	0.82
2:L:692:PRO:HA	6:L:2005:HOH:O	1.80	0.80
1:A:263:GLU:HA	1:A:266:GLU:OE1	1.81	0.80
1:E:339:PHE:HB3	1:E:340:PRO:HD3	1.63	0.80
1:D:279:LEU:H	1:D:279:LEU:HD12	1.47	0.80
1:A:247:LYS:HG3	1:A:266:GLU:OE2	1.82	0.79
1:D:16:ARG:HD3	1:D:155:ASN:HD21	1.46	0.79
1:B:31:HIS:HE1	1:B:52:ASN:HD22	1.28	0.79
1:B:247:LYS:HG3	1:B:266:GLU:OE2	1.81	0.79
1:D:248:VAL:O	1:D:250:ILE:HG13	1.82	0.79
1:G:67:MET:HG2	1:G:95:LEU:HD23	1.63	0.79
1:C:59:PRO:HD2	2:L:701:LEU:HD11	1.64	0.78
1:A:261:GLN:HE21	1:A:265:ILE:CD1	1.96	0.78
1:D:332:GLU:HG2	1:D:336:ARG:HH12	1.49	0.77
1:F:161:PRO:HA	1:F:166:GLN:OE1	1.85	0.77
1:H:135:GLU:HG3	1:H:147:PHE:CD1	2.19	0.77
1:D:161:PRO:HA	1:D:166:GLN:NE2	1.99	0.77
1:F:328:TRP:HZ3	1:F:330:ASP:HB3	1.48	0.77
1:A:226:VAL:HG12	6:A:2104:HOH:O	1.84	0.77
1:A:339:PHE:HB3	1:A:340:PRO:HD3	1.67	0.77
1:F:339:PHE:HB3	1:F:340:PRO:HD3	1.67	0.76
1:E:235:ALA:CB	1:E:336:ARG:HB2	2.15	0.76
1:A:261:GLN:NE2	1:A:265:ILE:HD11	1.99	0.76
1:B:155:ASN:H	1:B:155:ASN:ND2	1.83	0.76
1:F:182:ASP:HA	1:F:244:GLN:NE2	2.00	0.76
1:F:82:THR:HG22	6:F:2054:HOH:O	1.84	0.76
1:D:339:PHE:HB3	1:D:340:PRO:HD3	1.68	0.75
1:F:262:LEU:O	1:F:266:GLU:HG3	1.87	0.74
1:G:335:ALA:O	1:G:340:PRO:HD3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:HG11	1:D:262:LEU:HD22	1.70	0.73
1:B:262:LEU:O	1:B:266:GLU:HG3	1.88	0.73
1:D:24:VAL:HA	2:L:709:PRO:HG3	1.70	0.73
1:G:201:LEU:HG	6:G:2018:HOH:O	1.88	0.73
1:A:252:VAL:O	1:A:254:ILE:HG23	1.88	0.72
1:E:316:ARG:HB2	1:E:316:ARG:HH11	1.53	0.72
1:B:263:GLU:O	1:B:267:VAL:HG23	1.89	0.72
1:F:248:VAL:HG23	1:F:266:GLU:HG2	1.69	0.72
1:B:38:SER:HA	1:B:57:GLN:HE21	1.55	0.72
1:A:265:ILE:HG23	1:A:269:PHE:CE1	2.24	0.71
1:A:18:ALA:O	1:A:22:ILE:HG13	1.90	0.71
1:A:255:PRO:HB3	6:A:2055:HOH:O	1.90	0.71
1:A:45:GLU:HB3	6:A:2020:HOH:O	1.91	0.71
1:B:89:ILE:HD12	6:B:2059:HOH:O	1.88	0.71
1:H:335:ALA:O	1:H:340:PRO:HD3	1.90	0.71
1:F:195:ASP:OD1	1:F:328:TRP:HA	1.90	0.70
1:G:239:ARG:HG2	6:G:2157:HOH:O	1.90	0.70
2:P:686:ARG:HA	2:P:691:GLN:O	1.91	0.70
1:F:127:MET:HB2	1:F:261:GLN:NE2	2.06	0.70
1:A:320:GLU:HG3	6:A:2130:HOH:O	1.91	0.70
1:F:275:PRO:HA	6:F:2144:HOH:O	1.92	0.70
1:G:84:GLN:H	1:G:84:GLN:NE2	1.88	0.70
1:G:41:GLY:HA3	6:G:2025:HOH:O	1.92	0.70
1:B:31:HIS:CE1	1:B:52:ASN:HD22	2.09	0.69
1:A:161:PRO:HA	1:A:166:GLN:NE2	2.07	0.69
2:J:685:ARG:HD2	2:J:695:ASN:HA	1.72	0.69
1:H:115:ASP:HB3	1:H:118:LEU:HD12	1.75	0.69
1:H:348:LEU:HB3	1:H:350:TRP:HD1	1.56	0.69
1:A:165:PHE:HA	1:A:177:TRP:HE1	1.57	0.69
1:B:135:GLU:HG3	1:B:147:PHE:CD1	2.27	0.69
1:D:127:MET:HB2	1:D:261:GLN:NE2	2.06	0.69
2:N:683:LEU:HD12	2:N:684:TRP:N	2.07	0.69
1:A:235:ALA:O	1:A:236:LEU:HD23	1.93	0.69
1:F:45:GLU:O	1:F:48:GLN:HB3	1.92	0.69
1:F:224:SER:N	1:F:227:GLN:HE21	1.86	0.69
1:H:183:PRO:HD3	1:H:244:GLN:HG3	1.74	0.69
1:H:6:LYS:HE2	1:H:106:GLN:HE22	1.59	0.68
1:B:31:HIS:ND1	1:B:52:ASN:HB3	2.09	0.68
1:F:24:VAL:O	1:F:28:VAL:HG13	1.93	0.68
2:N:687:ASN:ND2	2:N:691:GLN:HB2	2.00	0.68
1:A:59:PRO:HD2	2:K:701:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:THR:CG2	1:F:239:ARG:HB3	2.24	0.68
1:A:342:GLU:O	1:A:346:ASN:HB2	1.92	0.68
1:C:48:GLN:HB2	1:C:55:LEU:HD12	1.76	0.68
1:G:202:GLN:HG2	1:G:324:LEU:O	1.94	0.68
2:K:686:ARG:HG2	2:K:687:ASN:H	1.57	0.68
2:N:688:PRO:HD3	6:N:2008:HOH:O	1.94	0.68
1:B:35:GLN:HG3	1:B:66:LEU:HD21	1.77	0.67
2:P:685:ARG:HE	2:P:695:ASN:HD22	1.41	0.67
1:A:349:ASP:HB2	1:A:352:LEU:HD12	1.76	0.67
1:C:333:GLU:HG3	2:K:680:THR:HB	1.76	0.67
1:E:20:SER:O	1:E:24:VAL:HG22	1.95	0.67
1:G:339:PHE:HB3	1:G:340:PRO:HD3	1.74	0.66
1:F:328:TRP:CZ3	1:F:330:ASP:HB3	2.29	0.66
1:A:347:GLY:O	1:A:348:LEU:HD23	1.95	0.66
1:D:135:GLU:HG3	1:D:147:PHE:CD1	2.30	0.66
2:M:685:ARG:HB2	2:M:693:LEU:HB2	1.78	0.66
1:D:333:GLU:HG3	2:L:680:THR:HB	1.76	0.66
1:H:178:HIS:HA	1:H:243:VAL:O	1.95	0.66
1:F:178:HIS:HA	1:F:243:VAL:O	1.95	0.66
1:A:254:ILE:HB	1:A:255:PRO:HD2	1.77	0.66
1:B:22:ILE:HG12	1:B:32:VAL:HG11	1.76	0.66
1:G:135:GLU:HG3	1:G:147:PHE:CD1	2.31	0.66
1:E:41:GLY:HA3	6:E:2032:HOH:O	1.96	0.66
1:B:275:PRO:O	1:B:278:PRO:HD3	1.96	0.65
1:G:24:VAL:O	1:G:28:VAL:HG22	1.96	0.65
1:B:7:THR:H	1:B:75:HIS:CD2	2.09	0.65
1:C:206:ASP:HB3	1:C:210:LYS:HD3	1.77	0.65
1:C:319:ASP:HB2	6:C:2170:HOH:O	1.95	0.65
1:A:261:GLN:O	1:A:265:ILE:HG13	1.96	0.65
1:H:235:ALA:HB1	1:H:336:ARG:HB2	1.79	0.65
2:P:711:SER:O	2:P:712:LEU:HB2	1.95	0.65
1:B:209:GLN:H	1:B:209:GLN:NE2	1.95	0.65
1:A:161:PRO:HA	1:A:166:GLN:HE21	1.62	0.65
1:C:343:GLU:OE1	1:C:348:LEU:HD13	1.96	0.65
1:E:235:ALA:HA	1:E:336:ARG:HD2	1.79	0.65
1:E:335:ALA:O	1:E:340:PRO:HD3	1.97	0.65
1:A:263:GLU:O	1:A:267:VAL:HG23	1.96	0.65
1:D:7:THR:H	1:D:75:HIS:HD2	1.45	0.65
1:A:182:ASP:HA	1:A:244:GLN:NE2	2.12	0.65
1:E:211:TRP:CZ2	1:E:324:LEU:HD21	2.32	0.64
1:A:170:MET:HB3	1:A:171:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ARG:HG3	1:D:317:VAL:N	2.12	0.64
1:D:248:VAL:HG23	1:D:266:GLU:HG2	1.79	0.64
1:H:224:SER:H	1:H:227:GLN:NE2	1.95	0.64
1:D:275:PRO:HA	6:D:2155:HOH:O	1.98	0.64
1:A:166:GLN:OE1	1:A:168:GLU:HB2	1.98	0.63
1:F:329:ARG:HG3	1:F:333:GLU:HB3	1.79	0.63
1:G:182:ASP:HB2	1:G:273:LYS:HE3	1.80	0.63
2:J:702:LYS:HE2	6:J:2012:HOH:O	1.97	0.63
1:F:7:THR:H	1:F:75:HIS:HD2	1.45	0.63
1:G:170:MET:HB2	1:G:172:ASP:OD2	1.98	0.63
1:A:52:ASN:N	6:A:2022:HOH:O	2.21	0.63
1:D:263:GLU:O	1:D:267:VAL:HG23	1.97	0.63
1:E:64:VAL:HG22	1:E:65:PRO:HD3	1.79	0.63
1:H:67:MET:HG2	1:H:95:LEU:HD23	1.79	0.63
1:H:89:ILE:HG22	1:H:93:LYS:HE2	1.80	0.63
1:E:235:ALA:HB1	1:E:336:ARG:CB	2.23	0.63
1:A:61:LEU:HD23	2:K:688:PRO:HB3	1.81	0.63
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.13	0.63
1:B:178:HIS:CD2	1:B:243:VAL:HB	2.33	0.63
1:B:265:ILE:HG23	1:B:269:PHE:CD1	2.33	0.62
1:E:178:HIS:HA	1:E:243:VAL:O	1.99	0.62
1:A:183:PRO:HD3	1:A:244:GLN:NE2	2.14	0.62
1:B:333:GLU:HG3	2:J:680:THR:HB	1.80	0.62
1:D:39:LEU:H	1:D:57:GLN:NE2	1.96	0.62
2:N:683:LEU:HD12	2:N:684:TRP:H	1.62	0.62
1:D:7:THR:H	1:D:75:HIS:CD2	2.17	0.62
2:K:689:GLU:O	2:K:689:GLU:HG2	2.00	0.62
1:C:192:ALA:HA	1:C:196:VAL:HG23	1.80	0.62
2:J:695:ASN:O	2:J:699:LEU:HB2	1.98	0.62
1:A:343:GLU:HB3	1:A:350:TRP:HE1	1.64	0.62
1:H:339:PHE:HB3	1:H:340:PRO:HD3	1.81	0.62
1:A:7:THR:H	1:A:75:HIS:CD2	2.17	0.62
1:B:144:PRO:HA	1:B:212:ASN:HD21	1.65	0.61
1:E:208:PRO:O	1:E:212:ASN:HB2	2.00	0.61
1:A:264:ALA:O	1:A:268:VAL:HG23	2.01	0.61
1:E:333:GLU:HG3	2:M:680:THR:HB	1.83	0.61
1:D:161:PRO:HA	1:D:166:GLN:HE21	1.65	0.61
1:F:24:VAL:HG12	1:F:201:LEU:HD11	1.82	0.61
1:C:59:PRO:HG2	1:C:63:ASN:HD22	1.65	0.61
1:C:159:SER:HB2	6:C:2108:HOH:O	2.01	0.61
1:E:101:ARG:HG3	6:E:2081:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:THR:HB	1:F:239:ARG:O	2.00	0.60
2:J:687:ASN:OD1	2:J:689:GLU:HB3	2.01	0.60
1:C:4:GLN:O	1:C:6:LYS:HD2	2.00	0.60
1:F:166:GLN:HE22	1:F:251:LYS:NZ	2.00	0.60
1:C:339:PHE:HB3	1:C:340:PRO:HD3	1.82	0.60
2:N:709:PRO:O	2:N:710:LEU:HD23	2.01	0.60
1:F:259:ARG:O	1:F:263:GLU:HG3	2.02	0.60
1:B:145:SER:H	1:B:212:ASN:ND2	1.99	0.60
1:A:194:HIS:HE1	1:A:327:GLY:O	1.83	0.60
2:N:673:CYS:O	2:N:677:PHE:HA	2.02	0.60
1:A:135:GLU:HG3	1:A:147:PHE:CE1	2.37	0.60
1:C:316:ARG:HD3	1:C:317:VAL:N	2.16	0.60
1:F:125:VAL:HG12	1:F:261:GLN:OE1	2.02	0.60
1:G:66:LEU:C	1:G:66:LEU:HD23	2.23	0.59
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.67	0.59
1:D:335:ALA:O	1:D:340:PRO:HD3	2.02	0.59
1:H:24:VAL:HG13	1:H:201:LEU:HD11	1.83	0.59
1:D:42:LEU:HB2	6:D:2033:HOH:O	2.01	0.59
1:D:262:LEU:O	1:D:266:GLU:HG3	2.02	0.59
1:G:248:VAL:O	1:G:250:ILE:HD12	2.02	0.59
1:E:178:HIS:CD2	1:E:243:VAL:HB	2.36	0.59
1:E:195:ASP:OD1	1:E:328:TRP:HA	2.02	0.59
1:H:255:PRO:HA	6:H:2143:HOH:O	2.01	0.59
1:H:174:THR:HB	6:H:2112:HOH:O	2.03	0.59
1:A:7:THR:H	1:A:75:HIS:HD2	1.51	0.59
1:D:320:GLU:OE2	1:D:320:GLU:HA	2.03	0.59
1:H:195:ASP:OD1	1:H:328:TRP:HA	2.03	0.59
1:A:145:SER:O	1:A:212:ASN:HA	2.03	0.59
1:F:183:PRO:HD3	1:F:244:GLN:NE2	2.17	0.58
1:G:84:GLN:NE2	1:G:84:GLN:N	2.51	0.58
1:H:264:ALA:O	1:H:268:VAL:HG23	2.03	0.58
1:E:202:GLN:HG2	1:E:324:LEU:O	2.03	0.58
1:B:24:VAL:HG23	1:B:25:ALA:N	2.18	0.58
1:H:66:LEU:C	1:H:66:LEU:HD23	2.24	0.58
1:B:120:GLY:C	1:B:122:TRP:H	2.06	0.58
1:D:16:ARG:CD	1:D:155:ASN:HD21	2.17	0.58
1:D:325:TRP:CZ3	2:L:699:LEU:HD22	2.37	0.58
1:H:166:GLN:HE22	1:H:251:LYS:NZ	2.02	0.58
1:A:201:LEU:O	1:A:205:LYS:HG3	2.02	0.58
1:C:24:VAL:HG21	1:C:198:PRO:HD3	1.86	0.58
1:C:224:SER:OG	1:C:227:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:GLU:OE1	1:F:348:LEU:HD12	2.03	0.58
1:B:13:ALA:HB3	1:B:36:VAL:HG12	1.86	0.58
1:F:174:THR:HG22	1:F:239:ARG:HB3	1.84	0.58
1:D:329:ARG:HG3	1:D:333:GLU:CD	2.24	0.58
1:C:174:THR:HG23	1:C:239:ARG:O	2.03	0.57
1:D:201:LEU:O	1:D:205:LYS:HG3	2.02	0.57
2:P:685:ARG:HE	2:P:695:ASN:ND2	2.01	0.57
1:B:226:VAL:HG21	6:B:2118:HOH:O	2.03	0.57
1:D:343:GLU:HB3	1:D:348:LEU:HD12	1.86	0.57
1:A:175:PHE:HB2	1:A:240:VAL:HG22	1.85	0.57
1:D:60:LEU:HD12	6:D:2065:HOH:O	2.04	0.57
1:H:134:VAL:O	1:H:138:VAL:HG23	2.03	0.57
1:G:169:LEU:HD12	1:G:174:THR:O	2.04	0.57
1:F:232:PHE:HB3	1:F:240:VAL:HG21	1.87	0.57
1:G:41:GLY:HA2	6:G:2024:HOH:O	2.03	0.57
1:D:121:PRO:HD2	6:D:2097:HOH:O	2.05	0.57
1:A:129:ALA:HB3	1:A:130:PRO:HD3	1.86	0.57
1:C:248:VAL:HG11	1:C:262:LEU:HD22	1.87	0.57
1:D:263:GLU:HA	1:D:266:GLU:CD	2.25	0.57
1:A:265:ILE:HG23	1:A:269:PHE:CD1	2.40	0.56
1:C:263:GLU:O	1:C:267:VAL:HG23	2.05	0.56
1:H:153:TYR:HB2	1:H:156:ASN:ND2	2.20	0.56
1:A:13:ALA:HB1	1:A:47:LEU:HD13	1.87	0.56
1:C:267:VAL:HG12	1:C:272:HIS:CD2	2.40	0.56
1:G:39:LEU:H	1:G:57:GLN:NE2	2.03	0.56
1:H:166:GLN:HE22	1:H:251:LYS:HZ2	1.53	0.56
1:A:89:ILE:HG13	1:A:130:PRO:HB3	1.87	0.56
1:B:37:HIS:HB3	6:B:2026:HOH:O	2.04	0.56
1:C:7:THR:H	1:C:75:HIS:HD2	1.51	0.56
1:C:202:GLN:HG3	1:C:324:LEU:O	2.05	0.56
1:H:104:THR:HB	6:H:2055:HOH:O	2.05	0.56
1:A:250:ILE:HD12	1:A:250:ILE:N	2.21	0.56
1:B:316:ARG:HG3	1:B:316:ARG:HH11	1.71	0.56
1:C:87:ASP:HB3	6:C:2056:HOH:O	2.04	0.56
2:M:687:ASN:CG	2:M:688:PRO:HD2	2.26	0.56
1:C:195:ASP:OD1	1:C:328:TRP:HA	2.05	0.56
1:F:28:VAL:HG22	1:F:30:HIS:CD2	2.40	0.56
1:G:166:GLN:HG2	1:G:168:GLU:HB3	1.87	0.56
1:A:223:LEU:HD22	1:A:227:GLN:HB3	1.87	0.56
1:B:267:VAL:HG12	1:B:272:HIS:CD2	2.41	0.56
1:D:24:VAL:HG23	1:D:25:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LEU:HG	6:G:2024:HOH:O	2.06	0.56
1:A:265:ILE:O	1:A:269:PHE:HD1	1.89	0.56
1:B:129:ALA:N	1:B:130:PRO:HD2	2.20	0.56
1:E:19:ALA:O	1:E:23:ARG:HG3	2.05	0.56
1:F:182:ASP:HA	1:F:244:GLN:HE21	1.70	0.56
1:D:125:VAL:HG12	1:D:261:GLN:OE1	2.06	0.56
1:D:267:VAL:O	1:D:271:GLU:HB3	2.06	0.56
2:M:687:ASN:ND2	2:M:688:PRO:HD2	2.20	0.56
1:B:181:PHE:HB3	6:B:2114:HOH:O	2.06	0.56
1:F:166:GLN:HE22	1:F:251:LYS:HZ3	1.52	0.56
1:F:43:ILE:O	1:F:46:GLU:HB3	2.06	0.55
1:H:264:ALA:HA	6:H:2147:HOH:O	2.05	0.55
1:C:153:TYR:HB2	1:C:156:ASN:ND2	2.22	0.55
1:E:135:GLU:HG3	1:E:147:PHE:CD1	2.42	0.55
1:E:348:LEU:N	1:E:348:LEU:HD22	2.21	0.55
1:F:267:VAL:O	1:F:271:GLU:HB2	2.06	0.55
1:A:344:GLU:HB2	1:A:351:MET:HE2	1.88	0.55
1:B:83:SER:HB2	1:B:127:MET:CE	2.37	0.55
1:C:48:GLN:HB2	1:C:55:LEU:CD1	2.37	0.55
1:C:174:THR:HG22	1:C:175:PHE:N	2.20	0.55
2:N:687:ASN:HB2	2:N:691:GLN:H	1.72	0.55
1:C:174:THR:CG2	1:C:175:PHE:N	2.70	0.55
1:C:246:PRO:HA	6:C:2141:HOH:O	2.06	0.55
1:E:127:MET:HE3	1:E:258:TYR:HA	1.87	0.55
1:H:178:HIS:CD2	1:H:243:VAL:HB	2.42	0.55
1:C:260:GLU:HA	1:C:263:GLU:OE1	2.06	0.55
1:D:3:GLN:N	6:D:2002:HOH:O	2.38	0.55
1:F:10:VAL:O	1:F:34:ALA:HA	2.06	0.55
2:I:697:CYS:SG	2:I:708:ARG:NH2	2.80	0.55
2:P:687:ASN:OD1	2:P:691:GLN:HB2	2.07	0.55
1:D:26:ALA:CB	1:D:50:ILE:HG21	2.37	0.55
1:H:194:HIS:HE1	1:H:327:GLY:O	1.90	0.55
1:H:192:ALA:HA	1:H:196:VAL:HG23	1.88	0.55
2:J:711:SER:O	2:J:712:LEU:HB2	2.06	0.55
1:A:243:VAL:HG13	1:A:243:VAL:O	2.06	0.55
1:B:145:SER:O	1:B:212:ASN:HA	2.07	0.55
1:E:86:GLY:HA2	6:E:2069:HOH:O	2.06	0.55
1:F:7:THR:H	1:F:75:HIS:CD2	2.23	0.55
1:E:316:ARG:HB2	1:E:316:ARG:NH1	2.22	0.55
1:F:229:CYS:SG	1:F:240:VAL:HG12	2.47	0.55
1:B:183:PRO:O	1:B:225:PRO:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ALA:HB3	1:D:36:VAL:HG12	1.89	0.54
1:A:19:ALA:O	1:A:23:ARG:HG3	2.07	0.54
1:F:224:SER:N	1:F:227:GLN:NE2	2.44	0.54
2:I:687:ASN:O	2:I:689:GLU:N	2.40	0.54
2:J:690:GLY:HA3	6:J:2008:HOH:O	2.07	0.54
1:C:247:LYS:HB2	6:C:2144:HOH:O	2.07	0.54
2:N:687:ASN:HB3	2:N:688:PRO:HD2	1.89	0.54
1:A:120:GLY:C	1:A:122:TRP:H	2.10	0.54
1:D:100:LYS:HD2	1:D:141:LEU:HB3	1.88	0.54
1:D:316:ARG:HG2	1:D:316:ARG:HH11	1.71	0.54
1:E:82:THR:O	1:E:88:GLU:HG3	2.07	0.54
1:G:248:VAL:HG23	1:G:266:GLU:HG2	1.90	0.54
1:B:248:VAL:HG12	1:B:250:ILE:CD1	2.38	0.54
1:C:316:ARG:HD3	1:C:317:VAL:H	1.71	0.54
1:F:19:ALA:O	1:F:23:ARG:HG3	2.07	0.54
1:F:248:VAL:O	1:F:250:ILE:HG12	2.08	0.54
1:G:38:SER:HA	1:G:57:GLN:HE21	1.71	0.54
1:A:262:LEU:HD23	1:A:265:ILE:HD12	1.90	0.54
1:B:83:SER:HB2	1:B:127:MET:HE1	1.90	0.53
1:B:202:GLN:HG2	1:B:324:LEU:O	2.08	0.53
1:D:153:TYR:HB2	1:D:156:ASN:ND2	2.23	0.53
1:D:195:ASP:OD1	1:D:328:TRP:HA	2.07	0.53
2:K:687:ASN:CB	2:K:691:GLN:HB2	2.38	0.53
1:A:336:ARG:HG2	1:A:336:ARG:NH1	2.22	0.53
1:F:13:ALA:HB2	1:F:34:ALA:HB1	1.90	0.53
2:O:695:ASN:O	2:O:699:LEU:HB2	2.07	0.53
1:B:8:ILE:HG12	1:B:76:LEU:HD12	1.90	0.53
1:H:135:GLU:HG3	1:H:147:PHE:CE1	2.43	0.53
1:G:159:SER:OG	1:G:348:LEU:HD22	2.08	0.53
1:A:152:ILE:HA	6:A:2076:HOH:O	2.09	0.53
1:A:235:ALA:HB1	1:A:336:ARG:HB2	1.91	0.53
1:G:84:GLN:HE21	1:G:84:GLN:N	1.96	0.53
1:H:254:ILE:HD11	1:H:259:ARG:HG2	1.89	0.53
2:K:687:ASN:HB2	2:K:691:GLN:O	2.09	0.53
1:A:178:HIS:CE1	1:A:243:VAL:HG11	2.44	0.53
1:E:66:LEU:HD23	1:E:66:LEU:C	2.29	0.53
1:A:223:LEU:HA	1:A:227:GLN:NE2	2.24	0.53
1:B:338:VAL:HG12	1:B:342:GLU:HG3	1.89	0.53
1:E:230:ALA:O	1:E:233:SER:HB3	2.09	0.52
1:H:66:LEU:HD23	1:H:66:LEU:O	2.09	0.52
1:B:135:GLU:HG3	1:B:147:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:VAL:HA	6:D:2141:HOH:O	2.10	0.52
1:C:262:LEU:O	1:C:266:GLU:HG3	2.09	0.52
1:D:182:ASP:HB2	1:D:273:LYS:HZ1	1.72	0.52
1:F:276:TYR:N	6:F:2144:HOH:O	2.41	0.52
1:A:118:LEU:HB2	1:A:119:TYR:CE1	2.45	0.52
1:C:256:VAL:O	1:C:260:GLU:HG3	2.10	0.52
1:E:158:THR:OG1	1:E:160:LEU:HD13	2.09	0.52
1:G:349:ASP:HB2	1:G:352:LEU:HD12	1.90	0.52
1:H:76:LEU:HD22	1:H:204:PHE:CD2	2.45	0.52
2:K:683:LEU:C	2:K:683:LEU:HD23	2.28	0.52
1:B:182:ASP:O	1:B:225:PRO:HG2	2.09	0.52
1:E:343:GLU:HG3	1:E:350:TRP:HZ2	1.74	0.52
1:E:348:LEU:HB3	1:E:350:TRP:CD1	2.44	0.52
1:A:135:GLU:HG3	1:A:147:PHE:CD1	2.44	0.52
1:C:16:ARG:HD3	1:C:155:ASN:HD21	1.75	0.52
1:G:195:ASP:OD1	1:G:328:TRP:HA	2.08	0.52
1:C:178:HIS:CD2	1:C:243:VAL:HB	2.45	0.52
1:C:239:ARG:NH2	1:C:241:THR:HG21	2.24	0.52
1:C:66:LEU:C	1:C:66:LEU:HD23	2.29	0.52
1:C:164:LEU:HD11	1:C:181:PHE:CE2	2.45	0.52
1:G:316:ARG:HG3	1:G:316:ARG:HH11	1.74	0.52
1:F:250:ILE:HD11	1:F:262:LEU:HD13	1.91	0.52
1:E:64:VAL:N	1:E:65:PRO:CD	2.73	0.52
2:N:702:LYS:NZ	6:N:2011:HOH:O	2.43	0.52
1:D:19:ALA:O	1:D:23:ARG:HG3	2.10	0.51
1:D:248:VAL:HG23	1:D:266:GLU:CG	2.40	0.51
1:E:127:MET:HB2	1:E:261:GLN:NE2	2.25	0.51
1:F:24:VAL:HG13	2:N:700:PHE:CZ	2.45	0.51
1:B:339:PHE:N	1:B:340:PRO:HD2	2.26	0.51
1:G:3:GLN:N	6:G:2002:HOH:O	2.43	0.51
2:O:673:CYS:O	2:O:677:PHE:HA	2.10	0.51
1:A:6:LYS:NZ	6:A:2006:HOH:O	2.43	0.51
1:B:223:LEU:HD22	1:B:227:GLN:HB3	1.93	0.51
1:A:234:ARG:O	1:A:234:ARG:HG2	2.11	0.51
1:B:134:VAL:O	1:B:138:VAL:HG23	2.11	0.51
1:D:39:LEU:H	1:D:57:GLN:HE21	1.59	0.51
1:C:128:TRP:C	1:C:130:PRO:HD2	2.31	0.51
1:C:342:GLU:HA	6:C:2184:HOH:O	2.09	0.51
1:F:207:GLY:HA3	1:F:209:GLN:NE2	2.26	0.51
1:A:343:GLU:HG3	1:A:350:TRP:HZ2	1.76	0.51
1:D:32:VAL:HB	1:D:53:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:HG3	1:C:147:PHE:CD1	2.46	0.51
1:F:124:ALA:O	1:F:126:PRO:HD3	2.11	0.51
1:H:65:PRO:HA	6:H:2049:HOH:O	2.11	0.51
1:H:260:GLU:HA	1:H:263:GLU:OE1	2.11	0.51
2:I:687:ASN:C	2:I:689:GLU:H	2.14	0.51
1:E:137:TYR:CE1	1:E:141:LEU:HD11	2.45	0.51
1:B:316:ARG:HG3	1:B:316:ARG:NH1	2.26	0.50
1:D:89:ILE:O	1:D:93:LYS:HG3	2.11	0.50
1:D:256:VAL:O	1:D:260:GLU:HG3	2.11	0.50
1:F:166:GLN:NE2	1:F:251:LYS:NZ	2.59	0.50
1:D:280:PRO:HA	1:D:283:SER:HB3	1.93	0.50
1:H:267:VAL:HG12	1:H:272:HIS:CD2	2.46	0.50
1:B:270:GLY:HA3	6:B:2143:HOH:O	2.12	0.50
1:C:123:PRO:HB2	6:C:2085:HOH:O	2.11	0.50
1:F:66:LEU:C	1:F:66:LEU:HD23	2.31	0.50
1:C:210:LYS:HE3	1:C:211:TRP:CZ2	2.47	0.50
1:D:120:GLY:C	1:D:122:TRP:H	2.15	0.50
1:G:316:ARG:HG3	1:G:316:ARG:NH1	2.27	0.50
1:B:155:ASN:HB2	6:B:2101:HOH:O	2.11	0.50
1:E:160:LEU:N	1:E:160:LEU:HD12	2.27	0.50
1:E:261:GLN:O	1:E:265:ILE:HD13	2.10	0.50
1:A:192:ALA:HA	1:A:196:VAL:HG23	1.93	0.50
1:B:335:ALA:O	1:B:340:PRO:HD3	2.12	0.50
1:F:178:HIS:CD2	1:F:243:VAL:HB	2.46	0.50
1:A:13:ALA:HB3	1:A:36:VAL:HG13	1.94	0.50
1:C:239:ARG:CZ	1:C:241:THR:HG21	2.42	0.50
1:A:125:VAL:CG1	1:A:261:GLN:HE22	2.24	0.50
1:B:128:TRP:C	1:B:130:PRO:HD2	2.33	0.50
1:C:144:PRO:HA	1:C:212:ASN:OD1	2.12	0.50
1:G:164:LEU:HG	1:G:165:PHE:CE2	2.47	0.50
2:M:711:SER:O	2:M:712:LEU:HB2	2.12	0.50
1:B:75:HIS:HB3	1:B:106:GLN:NE2	2.27	0.50
1:E:168:GLU:O	1:E:175:PHE:HA	2.11	0.50
1:E:245:VAL:HG22	1:E:247:LYS:H	1.76	0.50
1:H:128:TRP:CZ3	1:H:269:PHE:HZ	2.30	0.50
2:I:687:ASN:HB3	2:I:691:GLN:HG2	1.93	0.50
1:B:13:ALA:HB3	1:B:36:VAL:CG1	2.42	0.49
1:B:329:ARG:HG3	1:B:333:GLU:HB3	1.94	0.49
1:F:196:VAL:O	1:F:200:LEU:HG	2.12	0.49
1:H:24:VAL:HG22	2:P:700:PHE:CE2	2.47	0.49
2:I:674:THR:HG21	2:I:691:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:690:GLY:HA3	6:N:2009:HOH:O	2.11	0.49
1:E:65:PRO:HA	6:E:2055:HOH:O	2.12	0.49
1:E:137:TYR:HE1	1:E:141:LEU:HD11	1.77	0.49
1:F:211:TRP:CE3	1:F:216:ILE:HD11	2.48	0.49
1:G:46:GLU:O	1:G:49:ALA:HB3	2.12	0.49
2:M:687:ASN:CB	2:M:691:GLN:HB2	2.38	0.49
1:A:13:ALA:HB3	1:A:36:VAL:CG1	2.43	0.49
1:B:45:GLU:HB2	6:B:2031:HOH:O	2.13	0.49
1:D:37:HIS:HB2	6:D:2030:HOH:O	2.11	0.49
1:F:42:LEU:HA	1:F:45:GLU:OE2	2.12	0.49
1:F:136:ASN:ND2	6:F:2083:HOH:O	2.45	0.49
1:C:318:THR:O	1:C:322:ARG:HG3	2.12	0.49
1:D:64:VAL:N	1:D:65:PRO:CD	2.75	0.49
1:E:44:ALA:HB2	6:E:2031:HOH:O	2.11	0.49
6:G:2203:HOH:O	2:O:680:THR:HG22	2.13	0.49
1:H:115:ASP:HA	1:H:129:ALA:HB2	1.93	0.49
1:E:28:VAL:HG12	1:E:28:VAL:O	2.13	0.49
1:B:261:GLN:O	1:B:265:ILE:HG13	2.12	0.49
2:L:671:THR:HB	6:L:2002:HOH:O	2.12	0.49
1:C:13:ALA:HB3	1:C:36:VAL:HG12	1.94	0.49
2:K:687:ASN:HB3	2:K:691:GLN:H	1.77	0.49
1:C:194:HIS:HE1	1:C:327:GLY:O	1.96	0.49
1:G:187:LEU:O	1:G:222:THR:HA	2.13	0.49
1:H:39:LEU:HG	1:H:57:GLN:OE1	2.13	0.49
1:A:72:GLU:HG2	1:C:4:GLN:HE22	1.78	0.49
1:A:127:MET:HB2	1:A:261:GLN:OE1	2.13	0.49
1:B:67:MET:CE	1:B:95:LEU:HG	2.42	0.49
1:C:335:ALA:O	1:C:340:PRO:HD3	2.13	0.49
1:E:210:LYS:HE3	1:E:211:TRP:CZ2	2.48	0.49
1:G:192:ALA:HA	1:G:196:VAL:HG23	1.93	0.49
1:H:126:PRO:HB2	6:H:2144:HOH:O	2.12	0.49
1:A:348:LEU:HB3	1:A:350:TRP:HD1	1.78	0.48
1:C:257:GLY:N	6:C:2149:HOH:O	2.37	0.48
1:F:96:ALA:HB1	1:F:141:LEU:HD12	1.95	0.48
2:K:686:ARG:CG	2:K:687:ASN:H	2.25	0.48
1:B:263:GLU:HA	1:B:266:GLU:OE1	2.14	0.48
1:C:169:LEU:HB2	1:C:175:PHE:CE1	2.48	0.48
1:A:188:PRO:HA	1:A:222:THR:HG22	1.95	0.48
1:D:8:ILE:HG12	1:D:76:LEU:HB2	1.95	0.48
1:D:165:PHE:HA	1:D:177:TRP:HE1	1.77	0.48
1:G:24:VAL:CG1	1:G:201:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ALA:O	1:A:340:PRO:HD3	2.14	0.48
1:B:267:VAL:HG12	1:B:272:HIS:NE2	2.29	0.48
1:D:244:GLN:OE1	1:D:245:VAL:N	2.47	0.48
1:D:316:ARG:HG2	1:D:316:ARG:NH1	2.28	0.48
1:H:317:VAL:HG22	1:H:317:VAL:O	2.13	0.48
1:A:134:VAL:O	1:A:138:VAL:HG23	2.13	0.48
1:C:215:ARG:HD2	1:C:281:GLU:OE2	2.13	0.48
1:D:263:GLU:HA	1:D:266:GLU:OE2	2.13	0.48
1:F:145:SER:O	1:F:212:ASN:HA	2.13	0.48
1:A:87:ASP:HA	6:A:2051:HOH:O	2.14	0.48
1:A:281:GLU:HG2	6:A:2127:HOH:O	2.13	0.48
1:C:199:ALA:O	1:C:203:ILE:HG13	2.14	0.48
1:E:125:VAL:HG12	1:E:261:GLN:OE1	2.13	0.48
2:J:699:LEU:HD22	2:J:703:LEU:HD11	1.96	0.48
2:M:685:ARG:N	2:M:693:LEU:O	2.43	0.48
1:D:212:ASN:O	6:D:2130:HOH:O	2.20	0.48
1:F:263:GLU:O	1:F:267:VAL:HG23	2.14	0.48
1:A:236:LEU:O	1:A:237:ASN:HB2	2.14	0.48
1:C:190:LEU:HD21	1:C:218:LEU:HD13	1.95	0.48
1:E:75:HIS:O	1:E:76:LEU:HD23	2.14	0.48
1:E:275:PRO:HA	6:E:2175:HOH:O	2.14	0.48
2:K:686:ARG:HG2	2:K:687:ASN:N	2.26	0.48
1:D:17:GLN:HB2	6:D:2019:HOH:O	2.13	0.48
1:D:120:GLY:HA3	6:D:2097:HOH:O	2.14	0.48
1:H:67:MET:HG2	1:H:95:LEU:CD2	2.44	0.48
1:H:252:VAL:HG22	1:H:253:ASN:N	2.29	0.48
1:C:348:LEU:HD21	6:C:2107:HOH:O	2.13	0.48
1:F:194:HIS:HB2	1:F:329:ARG:NH2	2.29	0.48
1:F:258:TYR:CE2	1:F:262:LEU:HG	2.49	0.48
1:H:139:ARG:HG2	6:H:2098:HOH:O	2.12	0.48
1:H:168:GLU:HB3	1:H:170:MET:HE1	1.95	0.48
2:M:673:CYS:O	2:M:677:PHE:HA	2.13	0.48
1:A:228:VAL:O	1:A:231:ALA:HB3	2.13	0.47
1:D:10:VAL:O	1:D:34:ALA:HA	2.14	0.47
1:G:10:VAL:HG12	1:G:11:VAL:N	2.29	0.47
1:A:182:ASP:HB2	1:A:273:LYS:HD2	1.95	0.47
1:D:320:GLU:HG3	6:D:2134:HOH:O	2.14	0.47
1:E:183:PRO:O	1:E:225:PRO:HD2	2.13	0.47
1:F:250:ILE:CD1	1:F:262:LEU:HD13	2.44	0.47
2:J:711:SER:O	2:J:712:LEU:CB	2.61	0.47
1:D:192:ALA:HA	1:D:196:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:HIS:O	1:F:76:LEU:HD23	2.14	0.47
1:H:175:PHE:HB2	1:H:240:VAL:HG22	1.97	0.47
1:E:160:LEU:HD12	1:E:160:LEU:H	1.80	0.47
1:A:182:ASP:HB3	1:A:185:ILE:HB	1.96	0.47
1:D:6:LYS:HB3	1:D:75:HIS:CD2	2.49	0.47
1:D:12:ASN:O	1:D:12:ASN:ND2	2.47	0.47
1:F:235:ALA:CB	1:F:336:ARG:HB2	2.35	0.47
1:G:137:TYR:HA	6:G:2104:HOH:O	2.15	0.47
1:H:223:LEU:HA	1:H:227:GLN:NE2	2.29	0.47
1:B:338:VAL:C	1:B:340:PRO:HD2	2.35	0.47
1:G:182:ASP:OD2	1:G:273:LYS:HE3	2.15	0.47
1:G:248:VAL:O	1:G:250:ILE:CD1	2.62	0.47
1:H:128:TRP:O	1:H:131:LYS:HB2	2.15	0.47
1:H:166:GLN:NE2	1:H:251:LYS:NZ	2.62	0.47
2:L:673:CYS:O	2:L:677:PHE:HA	2.14	0.47
1:A:346:ASN:ND2	6:A:2144:HOH:O	2.47	0.47
1:B:186:PRO:HD3	6:B:2119:HOH:O	2.15	0.47
1:C:19:ALA:O	1:C:23:ARG:HG3	2.14	0.47
1:C:211:TRP:CE3	1:C:216:ILE:HD11	2.49	0.47
1:D:171:PRO:C	1:D:173:GLY:H	2.17	0.47
1:E:100:LYS:HD2	1:E:141:LEU:HB3	1.95	0.47
1:E:115:ASP:HA	1:E:129:ALA:HB2	1.97	0.47
1:F:24:VAL:HG13	2:N:700:PHE:HZ	1.79	0.47
1:F:162:TYR:N	1:F:162:TYR:CD2	2.83	0.47
1:A:64:VAL:N	1:A:65:PRO:CD	2.78	0.47
1:B:155:ASN:ND2	6:B:2100:HOH:O	2.46	0.47
1:B:248:VAL:HG12	1:B:250:ILE:HD13	1.96	0.47
1:G:125:VAL:CG1	1:G:261:GLN:HE22	2.28	0.47
1:G:153:TYR:HB2	1:G:156:ASN:ND2	2.30	0.47
1:A:35:GLN:CG	1:A:66:LEU:HD21	2.39	0.47
1:A:62:ASN:HA	6:A:2030:HOH:O	2.14	0.47
1:C:234:ARG:HD2	1:F:234:ARG:O	2.15	0.47
6:C:2126:HOH:O	2:K:703:LEU:HB3	2.14	0.47
1:E:339:PHE:HB3	1:E:340:PRO:CD	2.42	0.47
1:E:351:MET:HG2	1:E:352:LEU:N	2.30	0.47
1:B:349:ASP:O	1:B:351:MET:N	2.48	0.47
1:E:352:LEU:OXT	1:E:352:LEU:CD1	2.55	0.47
1:B:31:HIS:CE1	1:B:52:ASN:ND2	2.82	0.46
1:D:13:ALA:HB3	1:D:36:VAL:CG1	2.45	0.46
1:D:279:LEU:HD12	1:D:279:LEU:N	2.22	0.46
1:H:125:VAL:HG12	1:H:261:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:686:ARG:HD2	2:P:690:GLY:O	2.16	0.46
1:B:59:PRO:O	1:B:63:ASN:ND2	2.44	0.46
1:G:61:LEU:HD22	1:G:85:ALA:O	2.15	0.46
1:G:325:TRP:HA	6:G:2199:HOH:O	2.14	0.46
2:K:687:ASN:ND2	2:K:688:PRO:HD2	2.30	0.46
1:B:194:HIS:HB2	1:B:329:ARG:NH2	2.30	0.46
1:C:87:ASP:CB	6:C:2056:HOH:O	2.62	0.46
1:G:343:GLU:HG3	1:G:350:TRP:HZ2	1.79	0.46
1:B:24:VAL:HG23	1:B:25:ALA:H	1.80	0.46
1:D:256:VAL:HG22	1:D:260:GLU:HG3	1.98	0.46
1:G:113:MET:HB2	1:G:131:LYS:HD2	1.98	0.46
1:H:161:PRO:HA	1:H:166:GLN:OE1	2.15	0.46
1:H:263:GLU:O	1:H:266:GLU:HG2	2.14	0.46
1:A:72:GLU:HG2	1:C:4:GLN:NE2	2.31	0.46
1:B:80:ASN:ND2	1:B:111:SER:HB3	2.31	0.46
1:C:183:PRO:HB3	1:C:242:TYR:CD2	2.50	0.46
1:C:336:ARG:HD2	2:K:680:THR:OG1	2.15	0.46
1:D:163:PRO:HG2	1:D:254:ILE:HG21	1.98	0.46
1:G:247:LYS:HB2	6:G:2164:HOH:O	2.15	0.46
1:H:224:SER:H	1:H:227:GLN:HE21	1.60	0.46
1:B:180:PRO:HA	1:B:245:VAL:O	2.16	0.46
1:C:48:GLN:NE2	6:C:2031:HOH:O	2.40	0.46
1:H:135:GLU:HG3	1:H:147:PHE:CG	2.50	0.46
1:B:245:VAL:CG1	1:B:246:PRO:HD2	2.46	0.46
1:C:178:HIS:HA	1:C:243:VAL:O	2.15	0.46
1:D:6:LYS:HB3	1:D:75:HIS:HD2	1.80	0.46
1:D:129:ALA:N	1:D:130:PRO:CD	2.79	0.46
1:F:21:LEU:HB2	1:F:200:LEU:HD12	1.97	0.46
1:G:4:GLN:HA	1:H:72:GLU:OE2	2.16	0.46
1:C:101:ARG:NH1	6:C:2068:HOH:O	2.48	0.46
1:C:170:MET:HB2	1:C:172:ASP:OD1	2.16	0.46
1:D:184:ASP:O	1:D:186:PRO:HD3	2.16	0.46
1:D:343:GLU:CB	1:D:348:LEU:HD12	2.45	0.46
1:E:43:ILE:HG22	1:E:47:LEU:HD11	1.97	0.46
1:E:248:VAL:HG11	1:E:262:LEU:HD13	1.97	0.46
1:F:211:TRP:HA	1:F:214:HIS:HD2	1.80	0.46
1:G:190:LEU:HD12	1:G:191:ASP:N	2.30	0.46
1:H:39:LEU:HG	1:H:57:GLN:CD	2.36	0.46
2:N:681:THR:OG1	2:N:682:PRO:HD2	2.16	0.46
1:C:82:THR:O	1:C:88:GLU:HG2	2.16	0.46
1:D:116:HIS:HE1	1:D:128:TRP:CE3	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:GLU:HG3	1:F:147:PHE:CD1	2.51	0.46
1:F:166:GLN:HE21	1:F:168:GLU:HB2	1.80	0.46
1:A:194:HIS:HB2	1:A:329:ARG:NH2	2.31	0.46
1:C:129:ALA:N	1:C:130:PRO:HD2	2.30	0.46
1:F:349:ASP:O	1:F:351:MET:N	2.49	0.46
1:H:13:ALA:HB2	1:H:34:ALA:HB1	1.98	0.46
2:K:691:GLN:HA	2:K:692:PRO:HD3	1.82	0.46
1:A:63:ASN:ND2	1:A:66:LEU:HB2	2.31	0.45
1:A:343:GLU:HG3	1:A:350:TRP:CZ2	2.50	0.45
1:B:113:MET:HE1	6:B:2098:HOH:O	2.15	0.45
1:C:6:LYS:H	1:C:30:HIS:CE1	2.34	0.45
1:G:43:ILE:O	1:G:47:LEU:HG	2.16	0.45
1:G:239:ARG:NH1	1:G:241:THR:OG1	2.49	0.45
1:H:7:THR:H	1:H:75:HIS:CD2	2.14	0.45
1:D:279:LEU:H	1:D:279:LEU:CD1	2.22	0.45
1:D:319:ASP:O	1:D:323:LYS:HG3	2.15	0.45
1:G:125:VAL:CG1	1:G:261:GLN:NE2	2.80	0.45
1:G:232:PHE:HB3	1:G:240:VAL:HG21	1.98	0.45
1:G:239:ARG:HD2	6:G:2155:HOH:O	2.16	0.45
1:H:208:PRO:HD2	1:H:209:GLN:OE1	2.16	0.45
1:A:83:SER:HA	1:A:88:GLU:HG3	1.99	0.45
1:A:97:ASP:O	1:A:101:ARG:HG3	2.16	0.45
1:B:127:MET:HG3	1:B:261:GLN:OE1	2.16	0.45
1:C:13:ALA:HB3	1:C:36:VAL:CG1	2.46	0.45
1:D:145:SER:O	1:D:212:ASN:HA	2.16	0.45
1:F:166:GLN:NE2	1:F:251:LYS:HZ2	2.15	0.45
1:G:19:ALA:O	1:G:23:ARG:HG3	2.16	0.45
1:G:125:VAL:HG11	1:G:128:TRP:CD2	2.51	0.45
2:I:676:CYS:SG	2:I:678:THR:HG22	2.56	0.45
1:C:164:LEU:HD11	1:C:181:PHE:HE2	1.82	0.45
1:C:248:VAL:HG23	1:C:266:GLU:HG2	1.98	0.45
1:D:136:ASN:ND2	6:D:2103:HOH:O	2.50	0.45
1:G:348:LEU:HA	6:G:2210:HOH:O	2.17	0.45
1:B:64:VAL:N	1:B:65:PRO:CD	2.79	0.45
1:B:209:GLN:H	1:B:209:GLN:CD	2.20	0.45
1:C:22:ILE:HG12	1:C:32:VAL:HG11	1.98	0.45
1:D:99:ALA:HB2	1:D:108:TYR:HE2	1.80	0.45
1:F:180:PRO:HA	1:F:245:VAL:O	2.16	0.45
1:F:275:PRO:HG2	1:F:278:PRO:HB3	1.99	0.45
1:G:123:PRO:HG2	1:G:268:VAL:HG23	1.98	0.45
1:A:221:GLU:OE1	1:A:331:MET:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HD2	1:A:333:GLU:HG2	1.98	0.45
1:C:216:ILE:HD13	1:C:324:LEU:HD11	1.98	0.45
1:E:45:GLU:O	1:E:48:GLN:HB3	2.17	0.45
1:F:50:ILE:HD13	6:F:2017:HOH:O	2.14	0.45
1:G:33:ARG:HG2	1:G:33:ARG:HH11	1.82	0.45
1:H:16:ARG:NH1	1:H:155:ASN:OD1	2.45	0.45
1:B:43:ILE:HB	6:B:2030:HOH:O	2.17	0.45
1:G:42:LEU:N	6:G:2024:HOH:O	2.29	0.45
1:G:123:PRO:HD2	1:G:268:VAL:HG22	1.98	0.45
1:A:194:HIS:ND1	1:A:195:ASP:OD1	2.37	0.45
1:C:208:PRO:O	1:C:212:ASN:HB2	2.16	0.45
1:D:10:VAL:HG21	1:D:22:ILE:HD11	1.99	0.45
1:E:10:VAL:HG21	1:E:22:ILE:HD11	1.97	0.45
1:G:144:PRO:HA	1:G:212:ASN:ND2	2.32	0.45
1:H:263:GLU:O	1:H:267:VAL:HG23	2.17	0.45
2:L:681:THR:OG1	2:L:682:PRO:HD2	2.17	0.45
1:G:179:ALA:O	1:G:244:GLN:HA	2.17	0.45
1:G:262:LEU:O	1:G:266:GLU:HG3	2.17	0.45
1:B:169:LEU:HB2	1:B:175:PHE:CE1	2.51	0.44
1:E:46:GLU:HG3	1:E:47:LEU:N	2.32	0.44
1:G:28:VAL:HG21	1:G:201:LEU:HD21	1.98	0.44
1:G:100:LYS:HD2	1:G:141:LEU:HB3	1.98	0.44
1:H:160:LEU:HD11	1:H:346:ASN:HB3	2.00	0.44
1:A:177:TRP:CE3	1:A:242:TYR:CD1	3.05	0.44
1:A:212:ASN:ND2	1:G:215:ARG:HH12	2.15	0.44
1:E:64:VAL:CG2	1:E:65:PRO:HD3	2.47	0.44
1:H:24:VAL:HG22	2:P:700:PHE:CZ	2.53	0.44
2:O:676:CYS:SG	2:O:678:THR:HG22	2.58	0.44
1:A:13:ALA:HB2	1:A:34:ALA:HB1	2.00	0.44
1:C:180:PRO:HA	1:C:245:VAL:O	2.17	0.44
1:F:120:GLY:O	1:F:122:TRP:N	2.40	0.44
1:H:189:TRP:CZ2	1:H:228:VAL:HG21	2.53	0.44
1:E:76:LEU:HD22	1:E:107:HIS:HB3	1.98	0.44
1:F:320:GLU:HG3	6:F:2113:HOH:O	2.17	0.44
2:J:687:ASN:O	2:J:689:GLU:N	2.50	0.44
2:J:708:ARG:NE	6:J:2015:HOH:O	2.50	0.44
1:A:338:VAL:HG12	1:A:342:GLU:HG3	1.99	0.44
1:B:316:ARG:HG3	6:B:2158:HOH:O	2.17	0.44
1:B:319:ASP:HB2	6:B:2159:HOH:O	2.18	0.44
1:C:316:ARG:HH11	1:C:317:VAL:HG12	1.83	0.44
1:E:189:TRP:CZ2	1:E:228:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ILE:HD13	6:F:2011:HOH:O	2.18	0.44
1:G:125:VAL:HB	1:G:128:TRP:HB2	1.99	0.44
2:L:686:ARG:HG2	2:L:686:ARG:HH11	1.83	0.44
1:D:46:GLU:O	1:D:49:ALA:HB3	2.18	0.44
1:G:123:PRO:HG2	1:G:268:VAL:CG2	2.48	0.44
1:H:13:ALA:HB3	1:H:36:VAL:HG13	2.00	0.44
1:A:179:ALA:HA	1:A:180:PRO:HD3	1.85	0.44
1:D:179:ALA:O	1:D:244:GLN:HA	2.18	0.44
1:H:115:ASP:HB3	1:H:118:LEU:CD1	2.46	0.44
1:H:221:GLU:OE1	1:H:330:ASP:HB2	2.18	0.44
1:A:205:LYS:HB3	1:A:205:LYS:HZ3	1.83	0.44
1:B:115:ASP:HB3	1:B:118:LEU:CD1	2.35	0.44
1:D:66:LEU:C	1:D:66:LEU:HD23	2.38	0.44
1:F:187:LEU:O	1:F:222:THR:HA	2.18	0.44
1:H:24:VAL:HG13	1:H:201:LEU:CD1	2.48	0.44
1:H:348:LEU:HB3	1:H:350:TRP:CD1	2.45	0.44
2:O:687:ASN:OD1	2:O:689:GLU:HB3	2.17	0.44
1:A:117:SER:HA	1:A:122:TRP:O	2.18	0.44
1:B:144:PRO:HA	1:B:212:ASN:ND2	2.30	0.44
1:C:233:SER:HB2	1:F:234:ARG:HB3	1.99	0.44
1:D:250:ILE:O	1:D:250:ILE:HG22	2.18	0.44
1:E:192:ALA:HA	1:E:196:VAL:HG23	2.00	0.44
1:E:224:SER:OG	1:E:227:GLN:HG3	2.18	0.44
1:A:119:TYR:CD1	1:A:119:TYR:N	2.86	0.43
1:C:190:LEU:HD22	1:C:218:LEU:O	2.18	0.43
1:F:43:ILE:O	1:F:47:LEU:HG	2.18	0.43
1:H:202:GLN:HG2	1:H:324:LEU:O	2.18	0.43
1:C:64:VAL:N	1:C:65:PRO:CD	2.81	0.43
1:D:336:ARG:HD2	2:L:680:THR:OG1	2.19	0.43
1:E:343:GLU:OE2	1:E:343:GLU:HA	2.17	0.43
1:F:258:TYR:CD2	1:F:262:LEU:HG	2.53	0.43
1:G:50:ILE:HA	1:G:51:PRO:HD3	1.85	0.43
1:G:267:VAL:O	1:G:271:GLU:HB3	2.17	0.43
1:H:327:GLY:O	2:P:696:ALA:HB2	2.18	0.43
2:K:673:CYS:SG	2:K:693:LEU:HA	2.58	0.43
2:O:699:LEU:O	2:O:703:LEU:HG	2.17	0.43
1:A:178:HIS:CD2	1:A:249:GLU:OE1	2.71	0.43
1:B:178:HIS:HB2	6:B:2112:HOH:O	2.18	0.43
1:B:179:ALA:HB3	1:B:242:TYR:OH	2.18	0.43
1:E:245:VAL:HA	1:E:246:PRO:HD3	1.90	0.43
1:E:320:GLU:O	1:E:324:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG12	1:A:76:LEU:HB2	1.99	0.43
1:A:100:LYS:HB2	1:A:143:LEU:HD21	2.00	0.43
1:A:215:ARG:HD2	1:A:281:GLU:OE2	2.18	0.43
1:B:149:TYR:O	1:B:218:LEU:N	2.43	0.43
1:F:111:SER:HA	1:F:148:VAL:HG23	1.99	0.43
1:F:162:TYR:HA	1:F:163:PRO:HD3	1.89	0.43
1:G:336:ARG:HD2	2:O:680:THR:OG1	2.17	0.43
1:H:86:GLY:O	1:H:88:GLU:N	2.52	0.43
1:A:100:LYS:HG3	6:G:2029:HOH:O	2.19	0.43
1:A:202:GLN:HG2	1:A:324:LEU:O	2.19	0.43
1:B:39:LEU:H	1:B:57:GLN:NE2	2.17	0.43
1:D:61:LEU:HB2	1:D:91:ILE:HD11	2.00	0.43
1:D:135:GLU:HG3	1:D:147:PHE:CE1	2.53	0.43
1:E:129:ALA:HB3	1:E:130:PRO:HD3	1.99	0.43
1:H:23:ARG:NE	1:H:46:GLU:OE2	2.48	0.43
2:J:687:ASN:C	2:J:689:GLU:H	2.22	0.43
2:P:707:VAL:O	2:P:709:PRO:HD3	2.18	0.43
1:A:137:TYR:CZ	1:A:141:LEU:HD21	2.53	0.43
1:E:236:LEU:O	1:E:238:ARG:HG2	2.18	0.43
1:F:63:ASN:ND2	1:F:66:LEU:HB2	2.34	0.43
1:F:137:TYR:CE1	1:F:141:LEU:HD11	2.53	0.43
1:H:144:PRO:HA	1:H:212:ASN:OD1	2.18	0.43
1:H:224:SER:OG	1:H:227:GLN:HG3	2.17	0.43
1:A:201:LEU:HD13	2:I:704:HIS:CE1	2.54	0.43
1:D:144:PRO:HG3	6:D:2064:HOH:O	2.18	0.43
1:D:276:TYR:O	1:D:278:PRO:HD3	2.19	0.43
1:G:329:ARG:HD2	1:G:333:GLU:HG2	2.01	0.43
2:I:685:ARG:HD2	2:I:695:ASN:HA	1.99	0.43
2:I:687:ASN:C	2:I:689:GLU:N	2.72	0.43
2:K:683:LEU:HD23	2:K:684:TRP:N	2.33	0.43
2:O:699:LEU:HD22	2:O:703:LEU:CD1	2.48	0.43
1:A:258:TYR:O	1:A:262:LEU:HG	2.18	0.43
1:B:161:PRO:HB2	1:B:251:LYS:HB2	2.01	0.43
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.83	0.43
1:D:6:LYS:HE3	1:D:106:GLN:HE22	1.83	0.43
1:H:166:GLN:NE2	1:H:251:LYS:HZ1	2.17	0.43
2:K:700:PHE:HE1	2:K:706:VAL:HG23	1.84	0.43
1:A:343:GLU:CB	1:A:350:TRP:HE1	2.30	0.43
1:C:235:ALA:HB1	1:C:336:ARG:HB2	1.99	0.43
1:D:13:ALA:HB2	1:D:34:ALA:HB1	2.01	0.43
1:D:316:ARG:HG3	1:D:318:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:MET:HB2	1:F:261:GLN:HE22	1.83	0.43
1:D:168:GLU:O	1:D:175:PHE:HA	2.18	0.43
1:E:247:LYS:HD3	6:E:2170:HOH:O	2.19	0.43
2:I:691:GLN:HA	2:I:692:PRO:HD3	1.73	0.43
2:K:683:LEU:HD23	2:K:684:TRP:O	2.19	0.43
2:P:673:CYS:O	2:P:677:PHE:HA	2.19	0.43
1:A:223:LEU:HA	1:A:227:GLN:HE21	1.83	0.42
1:C:8:ILE:HG12	1:C:76:LEU:HB2	2.00	0.42
1:C:248:VAL:N	1:C:266:GLU:OE2	2.44	0.42
1:D:155:ASN:HA	1:D:334:TYR:OH	2.19	0.42
1:F:24:VAL:HG12	1:F:201:LEU:CD1	2.48	0.42
1:G:125:VAL:HG12	1:G:261:GLN:HE22	1.84	0.42
1:B:192:ALA:HA	1:B:196:VAL:HG23	2.01	0.42
1:C:185:ILE:HA	1:C:186:PRO:HD3	1.91	0.42
1:D:187:LEU:O	1:D:222:THR:HA	2.20	0.42
1:D:242:TYR:HB3	6:D:2142:HOH:O	2.18	0.42
1:F:17:GLN:HA	1:F:196:VAL:HG11	2.01	0.42
1:A:120:GLY:C	1:A:122:TRP:N	2.72	0.42
1:B:3:GLN:HA	6:B:2001:HOH:O	2.19	0.42
1:B:88:GLU:OE2	1:B:131:LYS:NZ	2.44	0.42
1:C:343:GLU:O	1:C:348:LEU:HB2	2.19	0.42
1:D:93:LYS:HE3	1:D:137:TYR:CD2	2.54	0.42
1:D:327:GLY:O	2:L:696:ALA:HB2	2.19	0.42
1:E:316:ARG:HG3	1:E:317:VAL:H	1.84	0.42
1:G:155:ASN:HA	1:G:334:TYR:CZ	2.54	0.42
1:G:234:ARG:HD3	1:G:332:GLU:OE1	2.18	0.42
1:H:64:VAL:N	1:H:65:PRO:CD	2.82	0.42
1:B:145:SER:N	1:B:212:ASN:ND2	2.65	0.42
1:B:195:ASP:OD1	1:B:328:TRP:HA	2.19	0.42
1:D:20:SER:OG	1:D:197:GLY:N	2.52	0.42
1:F:338:VAL:O	1:F:339:PHE:C	2.57	0.42
1:G:115:ASP:O	1:G:117:SER:N	2.52	0.42
1:G:175:PHE:CB	1:G:240:VAL:HG13	2.50	0.42
1:B:125:VAL:HG23	6:B:2079:HOH:O	2.18	0.42
1:B:152:ILE:HG12	1:B:276:TYR:CE2	2.54	0.42
1:B:188:PRO:HA	1:B:222:THR:HG22	2.00	0.42
1:C:269:PHE:HE2	1:C:276:TYR:HA	1.84	0.42
1:A:48:GLN:NE2	1:C:51:PRO:HG3	2.35	0.42
1:B:155:ASN:HA	1:B:334:TYR:OH	2.20	0.42
1:C:317:VAL:O	1:C:317:VAL:HG22	2.20	0.42
1:D:126:PRO:HG2	1:D:261:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:VAL:HG21	6:D:2076:HOH:O	2.20	0.42
1:E:126:PRO:HG2	1:E:261:GLN:HA	2.02	0.42
1:E:214:HIS:HE1	6:E:2153:HOH:O	2.03	0.42
1:F:174:THR:HG21	1:F:239:ARG:HB3	2.00	0.42
1:H:217:ALA:HB2	1:H:282:PHE:CE2	2.54	0.42
1:B:105:ILE:HG12	6:B:2075:HOH:O	2.20	0.42
1:D:121:PRO:HA	6:D:2093:HOH:O	2.19	0.42
1:D:207:GLY:HA3	1:D:209:GLN:HE22	1.85	0.42
1:F:208:PRO:C	1:F:210:LYS:H	2.22	0.42
1:G:235:ALA:CB	1:G:335:ALA:HB3	2.50	0.42
1:D:329:ARG:HG3	1:D:333:GLU:OE1	2.19	0.42
1:D:349:ASP:O	1:D:352:LEU:N	2.52	0.42
1:F:127:MET:HE2	6:F:2054:HOH:O	2.20	0.42
1:F:208:PRO:C	1:F:210:LYS:N	2.73	0.42
1:F:245:VAL:HG12	6:F:2126:HOH:O	2.19	0.42
1:G:3:GLN:NE2	1:G:3:GLN:HA	2.34	0.42
1:G:166:GLN:CG	1:G:168:GLU:HB3	2.49	0.42
2:L:681:THR:CB	2:L:694:CYS:HB2	2.49	0.42
1:A:317:VAL:HG13	1:A:318:THR:N	2.35	0.42
1:B:19:ALA:O	1:B:23:ARG:HG3	2.20	0.42
1:D:224:SER:N	1:D:227:GLN:OE1	2.38	0.42
1:E:125:VAL:HA	1:E:126:PRO:HD2	1.58	0.42
1:F:344:GLU:HB2	1:F:351:MET:HE2	2.01	0.42
1:H:192:ALA:HA	1:H:196:VAL:CG2	2.49	0.42
2:K:687:ASN:HB3	2:K:691:GLN:HB2	2.01	0.42
1:C:89:ILE:O	1:C:93:LYS:HG3	2.20	0.42
1:D:179:ALA:HA	1:D:180:PRO:HD3	1.83	0.42
1:E:134:VAL:O	1:E:138:VAL:HG23	2.20	0.42
1:E:209:GLN:CD	6:E:2147:HOH:O	2.58	0.42
1:G:159:SER:OG	1:G:348:LEU:CD2	2.68	0.42
1:G:168:GLU:OE1	1:G:251:LYS:NZ	2.53	0.42
1:H:153:TYR:CD1	1:H:192:ALA:HB2	2.55	0.42
1:B:245:VAL:HG13	1:B:246:PRO:HD2	2.01	0.41
1:D:12:ASN:O	1:D:12:ASN:CG	2.57	0.41
1:E:82:THR:C	1:E:88:GLU:HG3	2.39	0.41
1:F:64:VAL:N	1:F:65:PRO:CD	2.82	0.41
1:F:335:ALA:O	1:F:340:PRO:HD3	2.20	0.41
2:J:671:THR:HB	2:J:684:TRP:CE2	2.55	0.41
1:A:10:VAL:O	1:A:34:ALA:HA	2.20	0.41
1:B:10:VAL:HG11	1:B:18:ALA:HB1	2.03	0.41
1:B:174:THR:HG22	1:B:239:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:ILE:HA	1:F:51:PRO:HD3	1.87	0.41
1:G:51:PRO:HA	6:G:2035:HOH:O	2.20	0.41
2:O:687:ASN:O	2:O:689:GLU:N	2.53	0.41
1:C:164:LEU:HD12	1:C:164:LEU:O	2.20	0.41
1:D:52:ASN:HB2	6:D:2048:HOH:O	2.19	0.41
1:D:135:GLU:OE2	1:D:139:ARG:NH1	2.53	0.41
1:F:235:ALA:HB1	1:F:336:ARG:CB	2.38	0.41
1:H:256:VAL:O	1:H:260:GLU:HG3	2.20	0.41
2:K:687:ASN:ND2	2:K:688:PRO:CD	2.83	0.41
2:L:692:PRO:O	2:L:693:LEU:HD23	2.21	0.41
1:C:166:GLN:HG2	1:C:168:GLU:HB2	2.01	0.41
1:G:325:TRP:CZ3	2:O:699:LEU:HD13	2.55	0.41
2:J:671:THR:HB	2:J:684:TRP:CZ2	2.55	0.41
2:J:686:ARG:HB3	2:J:690:GLY:HA2	2.02	0.41
1:A:152:ILE:HG21	1:A:165:PHE:CZ	2.56	0.41
1:A:224:SER:H	1:A:227:GLN:NE2	2.19	0.41
1:A:329:ARG:HG3	1:A:333:GLU:HG2	2.02	0.41
1:B:100:LYS:HD2	1:B:141:LEU:HB3	2.01	0.41
1:E:67:MET:SD	1:E:94:ASP:HB3	2.60	0.41
1:E:144:PRO:HA	1:E:212:ASN:OD1	2.21	0.41
1:G:208:PRO:O	1:G:212:ASN:HB2	2.21	0.41
1:H:344:GLU:O	1:H:347:GLY:N	2.53	0.41
2:K:687:ASN:C	2:K:689:GLU:H	2.22	0.41
2:N:686:ARG:HB3	2:N:690:GLY:HA2	2.02	0.41
1:A:43:ILE:O	1:A:46:GLU:HB3	2.21	0.41
1:A:205:LYS:HB3	1:A:205:LYS:HZ2	1.83	0.41
1:A:260:GLU:HA	1:A:263:GLU:HG3	2.03	0.41
1:B:248:VAL:HG12	1:B:250:ILE:HD11	2.02	0.41
1:C:157:PHE:HA	1:C:165:PHE:O	2.21	0.41
1:C:225:PRO:HB3	1:C:242:TYR:CE1	2.56	0.41
1:E:10:VAL:O	1:E:34:ALA:HA	2.21	0.41
1:G:329:ARG:CZ	1:G:338:VAL:HG21	2.51	0.41
1:C:78:PHE:CZ	1:C:200:LEU:HD11	2.56	0.41
1:C:233:SER:O	1:C:237:ASN:N	2.54	0.41
1:H:321:ALA:O	1:H:324:LEU:HB2	2.21	0.41
2:K:710:LEU:O	2:K:711:SER:HB3	2.20	0.41
1:C:87:ASP:OD2	1:C:90:ALA:HB2	2.21	0.41
1:C:172:ASP:OD1	1:C:174:THR:HB	2.21	0.41
1:E:43:ILE:HG22	1:E:47:LEU:CD1	2.51	0.41
1:E:179:ALA:O	1:E:244:GLN:HA	2.21	0.41
1:E:275:PRO:HG2	1:E:278:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:MET:CG	1:H:95:LEU:HD23	2.49	0.41
1:H:128:TRP:HZ3	1:H:269:PHE:HZ	1.67	0.41
2:I:683:LEU:HD12	2:I:684:TRP:N	2.35	0.41
1:B:10:VAL:O	1:B:34:ALA:HA	2.21	0.41
1:C:80:ASN:O	1:C:80:ASN:CG	2.59	0.41
1:E:43:ILE:O	1:E:47:LEU:HG	2.21	0.41
1:E:348:LEU:HB3	1:E:350:TRP:HD1	1.84	0.41
1:F:172:ASP:OD2	1:F:173:GLY:N	2.54	0.41
1:G:41:GLY:O	1:G:45:GLU:HG3	2.20	0.41
2:K:681:THR:HA	2:K:682:PRO:HD3	1.92	0.41
2:L:676:CYS:O	2:L:677:PHE:HB2	2.21	0.41
2:M:676:CYS:HA	2:M:710:LEU:HD11	2.03	0.41
2:M:699:LEU:O	2:M:703:LEU:HG	2.21	0.41
1:B:16:ARG:HD3	1:B:155:ASN:OD1	2.21	0.41
1:C:187:LEU:O	1:C:222:THR:HA	2.21	0.41
1:D:208:PRO:O	1:D:212:ASN:HB2	2.21	0.41
1:E:335:ALA:HA	1:E:339:PHE:HB2	2.02	0.41
1:H:125:VAL:HA	1:H:126:PRO:HD2	1.76	0.41
1:H:323:LYS:HE2	6:H:2126:HOH:O	2.21	0.41
2:K:710:LEU:O	2:K:711:SER:CB	2.69	0.41
2:L:686:ARG:HA	6:L:2005:HOH:O	2.20	0.41
2:O:699:LEU:HD22	2:O:703:LEU:HG	2.03	0.41
1:A:100:LYS:HE3	6:G:2029:HOH:O	2.20	0.40
1:A:185:ILE:O	1:A:185:ILE:HG22	2.21	0.40
1:A:189:TRP:CZ2	1:A:228:VAL:HG21	2.55	0.40
1:C:125:VAL:HA	1:C:126:PRO:HD3	1.91	0.40
1:C:127:MET:HG3	1:C:261:GLN:OE1	2.21	0.40
1:D:155:ASN:HA	1:D:334:TYR:CZ	2.57	0.40
1:D:162:TYR:HA	1:D:163:PRO:HD3	1.89	0.40
2:P:674:THR:HG21	2:P:691:GLN:HE22	1.86	0.40
1:D:322:ARG:NH2	1:D:328:TRP:CH2	2.90	0.40
1:E:190:LEU:HD12	1:E:191:ASP:N	2.36	0.40
1:F:66:LEU:HD23	1:F:66:LEU:O	2.21	0.40
1:G:125:VAL:HA	1:G:126:PRO:HD2	1.79	0.40
1:A:229:CYS:SG	1:A:240:VAL:HG12	2.61	0.40
1:B:236:LEU:O	1:B:238:ARG:HG3	2.22	0.40
1:C:182:ASP:HB3	1:C:185:ILE:HD12	2.03	0.40
1:C:329:ARG:HG3	1:C:333:GLU:HB3	2.02	0.40
1:E:255:PRO:HB2	6:E:2164:HOH:O	2.20	0.40
2:J:679:GLN:OE1	2:J:679:GLN:N	2.54	0.40
1:D:160:LEU:O	1:D:166:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:HIS:CD2	1:D:329:ARG:HD3	2.56	0.40
1:E:145:SER:O	1:E:212:ASN:HA	2.22	0.40
1:F:10:VAL:HG21	1:F:22:ILE:HD11	2.02	0.40
1:G:316:ARG:HA	6:G:2189:HOH:O	2.21	0.40
1:G:318:THR:O	1:G:322:ARG:HG3	2.21	0.40
1:H:263:GLU:O	1:H:266:GLU:CG	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/352 (89%)	291 (93%)	20 (6%)	3 (1%)	15	32
1	B	314/352 (89%)	287 (91%)	24 (8%)	3 (1%)	15	32
1	C	314/352 (89%)	290 (92%)	22 (7%)	2 (1%)	25	47
1	D	314/352 (89%)	292 (93%)	19 (6%)	3 (1%)	15	32
1	E	314/352 (89%)	285 (91%)	27 (9%)	2 (1%)	25	47
1	F	314/352 (89%)	280 (89%)	33 (10%)	1 (0%)	41	64
1	G	314/352 (89%)	294 (94%)	18 (6%)	2 (1%)	25	47
1	H	314/352 (89%)	288 (92%)	21 (7%)	5 (2%)	9	19
2	I	40/43 (93%)	37 (92%)	2 (5%)	1 (2%)	5	9
2	J	40/43 (93%)	36 (90%)	3 (8%)	1 (2%)	5	9
2	K	39/43 (91%)	35 (90%)	3 (8%)	1 (3%)	5	9
2	L	40/43 (93%)	31 (78%)	8 (20%)	1 (2%)	5	9
2	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
2	N	40/43 (93%)	37 (92%)	3 (8%)	0	100	100
2	O	39/43 (91%)	37 (95%)	1 (3%)	1 (3%)	5	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	40/43 (93%)	38 (95%)	1 (2%)	1 (2%)	5 9
All	All	2831/3160 (90%)	2596 (92%)	208 (7%)	27 (1%)	15 32

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	TRP
1	G	116	HIS
1	A	253	ASN
1	B	319	ASP
1	F	350	TRP
1	H	87	ASP
1	H	116	HIS
1	A	172	ASP
1	C	51	PRO
1	D	251	LYS
1	D	350	TRP
1	G	51	PRO
1	H	51	PRO
2	I	688	PRO
2	K	686	ARG
1	E	51	PRO
2	L	711	SER
2	P	711	SER
1	A	51	PRO
1	B	51	PRO
1	D	51	PRO
2	J	688	PRO
1	C	126	PRO
1	H	234	ARG
1	E	126	PRO
1	H	126	PRO
2	O	688	PRO

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	266/284 (94%)	259 (97%)	7 (3%)	46	72
1	B	266/284 (94%)	261 (98%)	5 (2%)	57	79
1	C	266/284 (94%)	263 (99%)	3 (1%)	73	88
1	D	266/284 (94%)	257 (97%)	9 (3%)	37	63
1	E	266/284 (94%)	260 (98%)	6 (2%)	50	75
1	F	266/284 (94%)	261 (98%)	5 (2%)	57	79
1	G	266/284 (94%)	262 (98%)	4 (2%)	65	83
1	H	266/284 (94%)	259 (97%)	7 (3%)	46	72
2	I	38/39 (97%)	38 (100%)	0	100	100
2	J	38/39 (97%)	37 (97%)	1 (3%)	46	72
2	K	37/39 (95%)	36 (97%)	1 (3%)	44	71
2	L	38/39 (97%)	38 (100%)	0	100	100
2	M	39/39 (100%)	38 (97%)	1 (3%)	46	72
2	N	38/39 (97%)	38 (100%)	0	100	100
2	O	37/39 (95%)	34 (92%)	3 (8%)	11	23
2	P	38/39 (97%)	38 (100%)	0	100	100
All	All	2431/2584 (94%)	2379 (98%)	52 (2%)	53	77

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	36	VAL
1	A	184	ASP
1	A	225	PRO
1	A	252	VAL
1	A	316	ARG
1	A	351	MET
1	B	80	ASN
1	B	155	ASN
1	B	209	GLN
1	B	218	LEU
1	B	332	GLU
1	C	80	ASN
1	C	218	LEU
1	C	337	GLU
1	D	4	GLN

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Mol	Chain	Res	Type
1	D	12	ASN
1	D	31	HIS
1	D	51	PRO
1	D	122	TRP
1	D	209	GLN
1	D	244	GLN
1	D	342	GLU
1	D	349	ASP
1	E	40	LYS
1	E	45	GLU
1	E	51	PRO
1	E	155	ASN
1	E	212	ASN
1	E	351	MET
1	F	28	VAL
1	F	82	THR
1	F	155	ASN
1	F	237	ASN
1	F	351	MET
1	G	28	VAL
1	G	84	GLN
1	G	117	SER
1	G	316	ARG
1	H	24	VAL
1	H	36	VAL
1	H	167	MET
1	H	209	GLN
1	H	232	PHE
1	H	244	GLN
1	H	351	MET
2	J	699	LEU
2	K	687	ASN
2	M	687	ASN
2	O	671	THR
2	O	672	THR
2	O	699	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	52	ASN

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Mol	Chain	Res	Type
1	A	62	ASN
1	A	75	HIS
1	A	84	GLN
1	A	178	HIS
1	A	227	GLN
1	A	244	GLN
1	A	261	GLN
1	A	346	ASN
1	B	31	HIS
1	B	57	GLN
1	B	75	HIS
1	B	84	GLN
1	B	136	ASN
1	B	209	GLN
1	B	212	ASN
1	B	346	ASN
1	C	3	GLN
1	C	4	GLN
1	C	17	GLN
1	C	31	HIS
1	C	52	ASN
1	C	57	GLN
1	C	62	ASN
1	C	75	HIS
1	C	106	GLN
1	C	136	ASN
1	C	140	GLN
1	C	156	ASN
1	C	202	GLN
1	C	214	HIS
1	C	237	ASN
1	C	244	GLN
1	C	272	HIS
1	D	12	ASN
1	D	31	HIS
1	D	57	GLN
1	D	75	HIS
1	D	106	GLN
1	D	136	ASN
1	D	155	ASN
1	D	202	GLN
1	D	209	GLN

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Mol	Chain	Res	Type
1	D	346	ASN
1	E	52	ASN
1	E	57	GLN
1	E	62	ASN
1	E	75	HIS
1	E	106	GLN
1	E	136	ASN
1	E	178	HIS
1	E	244	GLN
1	E	346	ASN
1	F	3	GLN
1	F	62	ASN
1	F	75	HIS
1	F	84	GLN
1	F	106	GLN
1	F	136	ASN
1	F	156	ASN
1	F	166	GLN
1	F	178	HIS
1	F	227	GLN
1	F	237	ASN
1	F	244	GLN
1	F	253	ASN
1	G	3	GLN
1	G	4	GLN
1	G	52	ASN
1	G	57	GLN
1	G	84	GLN
1	G	107	HIS
1	G	136	ASN
1	G	156	ASN
1	G	166	GLN
1	G	244	GLN
1	G	272	HIS
1	H	52	ASN
1	H	62	ASN
1	H	84	GLN
1	H	106	GLN
1	H	136	ASN
1	H	156	ASN
1	H	166	GLN
1	H	227	GLN

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Mol	Chain	Res	Type
1	H	244	GLN
1	H	272	HIS
2	K	679	GLN
2	K	687	ASN
2	L	679	GLN
2	L	704	HIS
2	M	675	ASN
2	M	687	ASN
2	N	687	ASN
2	N	691	GLN
2	O	679	GLN
2	P	691	GLN
2	P	695	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	E	1353	-	4,4,4	0.29	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	1353	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	H	1353	-	4,4,4	0.26	0	6,6,6	0.21	0
3	SO4	B	1353	-	4,4,4	0.30	0	6,6,6	0.17	0
3	SO4	D	1353	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	G	1353	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	F	1353	-	4,4,4	0.26	0	6,6,6	0.22	0
3	SO4	A	1353	-	4,4,4	0.39	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	318/352 (90%)	-0.54	0 100 100	8, 28, 61, 91	0
1	B	318/352 (90%)	-0.53	0 100 100	9, 26, 53, 73	0
1	C	318/352 (90%)	-0.68	1 (0%) 94 93	10, 22, 45, 69	0
1	D	318/352 (90%)	-0.63	0 100 100	10, 26, 57, 72	0
1	E	318/352 (90%)	-0.57	0 100 100	8, 24, 52, 75	0
1	F	318/352 (90%)	-0.51	2 (0%) 89 88	9, 25, 55, 70	0
1	G	318/352 (90%)	-0.67	0 100 100	5, 23, 50, 75	0
1	H	318/352 (90%)	-0.63	0 100 100	7, 24, 59, 82	0
2	I	42/43 (97%)	-0.03	3 (7%) 16 11	8, 33, 92, 111	0
2	J	42/43 (97%)	-0.14	1 (2%) 59 53	14, 37, 89, 101	0
2	K	41/43 (95%)	-0.21	2 (4%) 29 23	12, 37, 100, 104	0
2	L	42/43 (97%)	-0.12	0 100 100	16, 41, 96, 119	0
2	M	43/43 (100%)	0.17	4 (9%) 8 6	13, 35, 101, 116	0
2	N	42/43 (97%)	-0.11	2 (4%) 30 24	9, 31, 90, 110	0
2	O	41/43 (95%)	-0.01	3 (7%) 15 11	20, 34, 89, 106	0
2	P	42/43 (97%)	0.03	4 (9%) 8 5	14, 39, 99, 107	0
All	All	2879/3160 (91%)	-0.53	22 (0%) 86 84	5, 26, 59, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	688	PRO	6.9
2	O	688	PRO	5.2
2	I	688	PRO	5.1
2	M	670	PRO	4.3
2	P	686	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	O	690	GLY	3.8
2	J	688	PRO	3.7
2	I	687	ASN	3.6
2	P	688	PRO	3.5
2	P	687	ASN	3.5
1	F	345	ALA	3.4
2	N	687	ASN	3.2
1	C	85	ALA	3.1
2	N	688	PRO	3.0
2	K	688	PRO	2.7
2	K	686	ARG	2.3
2	I	686	ARG	2.3
2	M	689	GLU	2.2
2	P	691	GLN	2.2
2	M	687	ASN	2.0
2	O	691	GLN	2.0
1	F	229	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1353	5/5	0.92	0.17	19,46,53,63	0
4	CL	A	1354	1/1	0.92	0.23	58,58,58,58	0
4	CL	F	1354	1/1	0.93	0.12	71,71,71,71	0
3	SO4	A	1353	5/5	0.94	0.13	30,31,52,71	0
3	SO4	F	1353	5/5	0.94	0.15	20,31,46,51	0
5	ZN	M	1713	1/1	0.95	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	D	1354	1/1	0.96	0.11	56,56,56,56	0
3	SO4	C	1353	5/5	0.96	0.12	25,29,58,59	0
4	CL	G	1354	1/1	0.96	0.10	37,37,37,37	0
3	SO4	E	1353	5/5	0.96	0.12	35,37,54,58	0
5	ZN	O	1712	1/1	0.96	0.19	57,57,57,57	0
3	SO4	G	1353	5/5	0.97	0.10	24,34,46,62	0
3	SO4	H	1353	5/5	0.97	0.12	38,51,57,63	0
3	SO4	D	1353	5/5	0.98	0.10	18,23,47,55	0
4	CL	H	1354	1/1	0.98	0.09	44,44,44,44	0
5	ZN	I	1713	1/1	0.99	0.11	38,38,38,38	0
5	ZN	J	1713	1/1	0.99	0.10	40,40,40,40	0
5	ZN	K	1712	1/1	0.99	0.12	30,30,30,30	0
5	ZN	L	1713	1/1	0.99	0.10	36,36,36,36	0
4	CL	G	1355	1/1	0.99	0.05	41,41,41,41	0
5	ZN	N	1713	1/1	0.99	0.11	34,34,34,34	0
4	CL	C	1354	1/1	0.99	0.12	49,49,49,49	0
5	ZN	P	1713	1/1	0.99	0.09	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.