Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:55 AM GMT

PDB ID	:	3NHQ
Title	:	The dark Pfr structure of the photosensory core module of P. aeruginosa Bacteriophytochrome
Authors	:	Yang, X.; Ren, Z.; Kuk, J.; Moffat, K.
Deposited on	:	2010-06-14
Resolution	:	2.55 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:

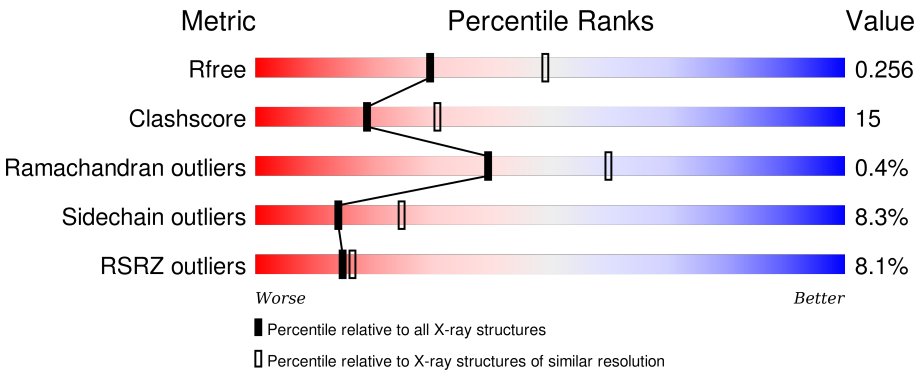
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	505	2%, 64%, 29%, • 5%
1	B	505	11%, 62%, 27%, • 7%
1	C	505	3%, 67%, 26%, • 5%
1	D	505	10%, 64%, 27%, • 5%
1	E	505	8%, 64%, 27%, • 5%

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Mol	Chain	Length	Quality of chain
1	F	505	11% 64% 25% 5% 7%
1	G	505	2% 65% 26% 5%
1	H	505	15% 64% 28% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30788 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3790	2386	682	703	19	0	0	0
1	B	470	3709	2332	665	693	19	0	0	0
1	C	482	3812	2398	688	707	19	0	0	0
1	D	480	3801	2391	686	705	19	0	0	0
1	E	479	3790	2386	683	702	19	0	0	0
1	F	471	3717	2338	666	694	19	0	0	0
1	G	482	3816	2401	688	708	19	0	1	0
1	H	481	3808	2396	687	706	19	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
A	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
A	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
B	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
B	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
C	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
C	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
D	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
D	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
E	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
E	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
F	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
F	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
G	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
G	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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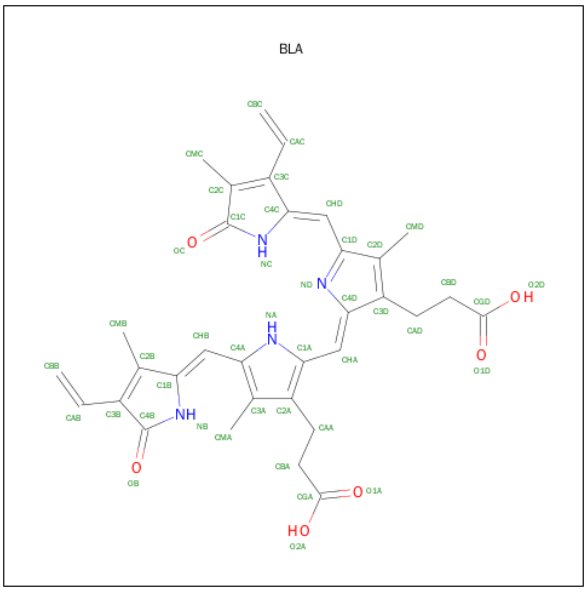
Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
H	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
H	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	43	33	4	6	0	0
2	B	1	43	33	4	6	0	0
2	C	1	43	33	4	6	0	0
2	D	1	43	33	4	6	0	0
2	E	1	43	33	4	6	0	0
2	F	1	43	33	4	6	0	0
2	G	1	43	33	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	H	1	43	33	4	6	0	0

- Molecule 3 is water.

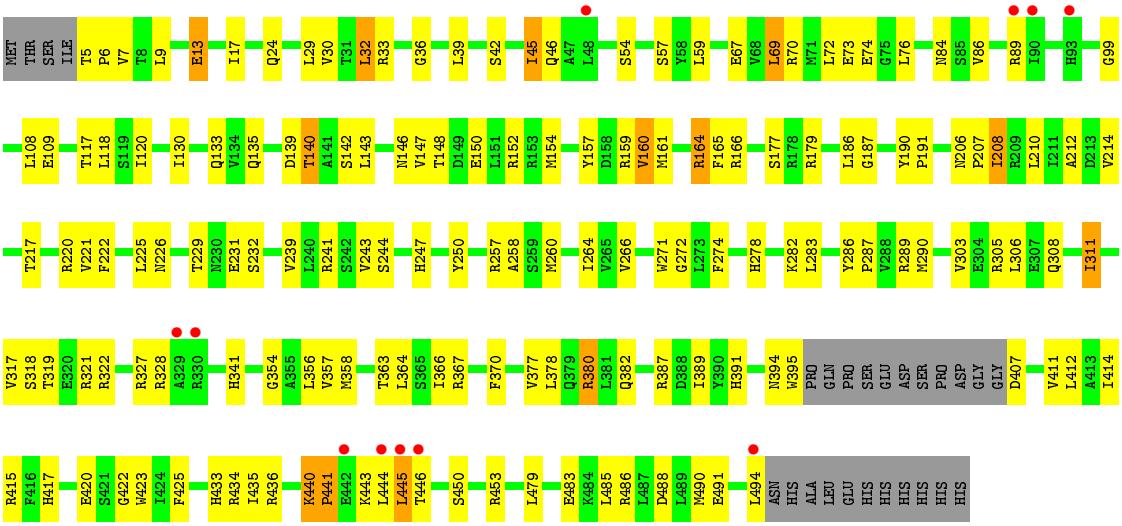
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	61	61	61	0	0
3	B	16	16	16	0	0
3	C	44	44	44	0	0
3	D	14	14	14	0	0
3	E	15	15	15	0	0
3	F	7	7	7	0	0
3	G	37	37	37	0	0
3	H	7	7	7	0	0

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.

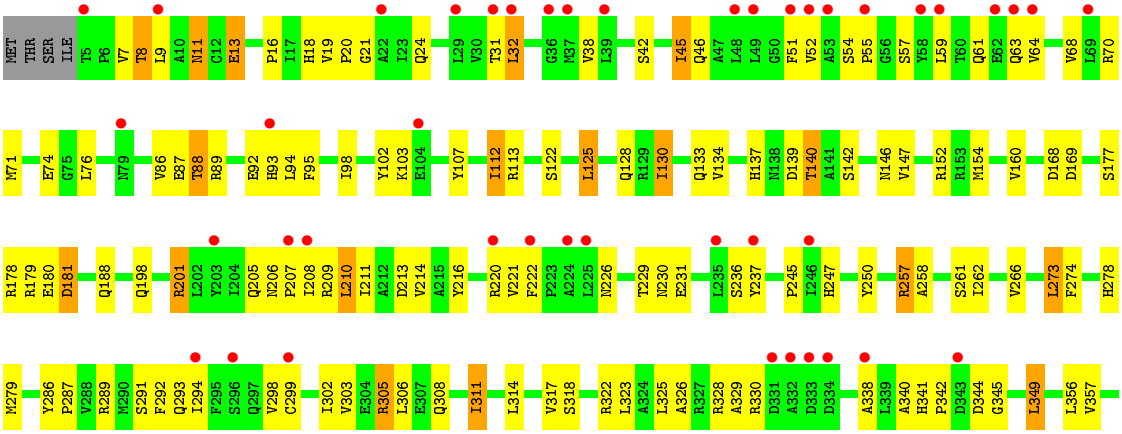
- Molecule 1: Bacteriophytochrome

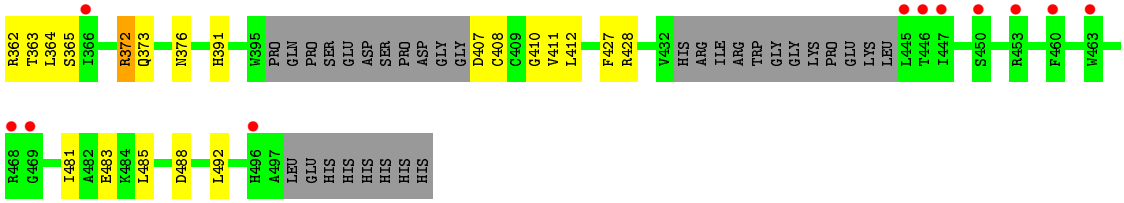
Chain A:



- Molecule 1: Bacteriophytochrome

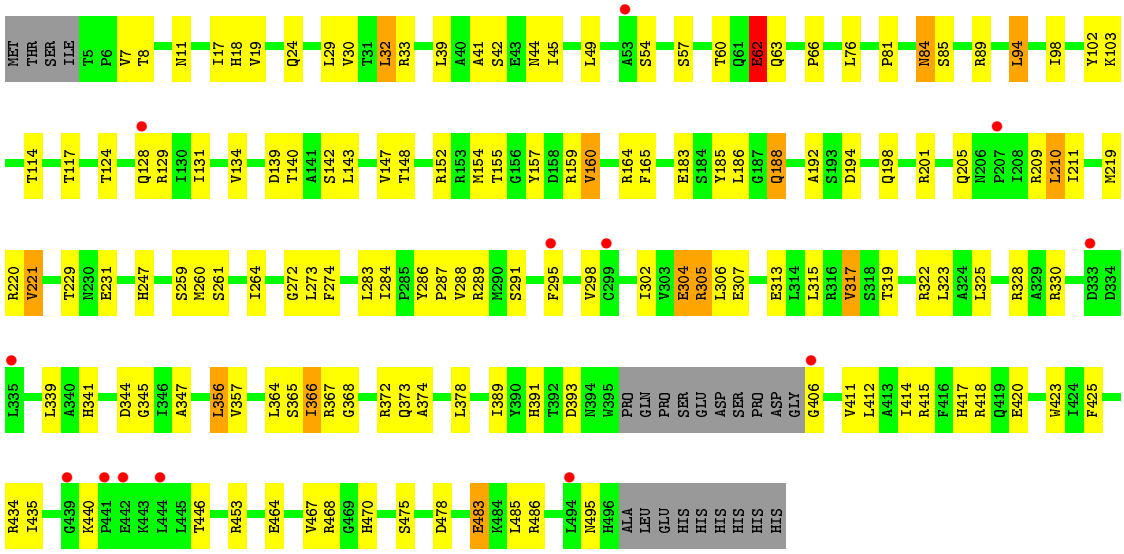
Chain B:





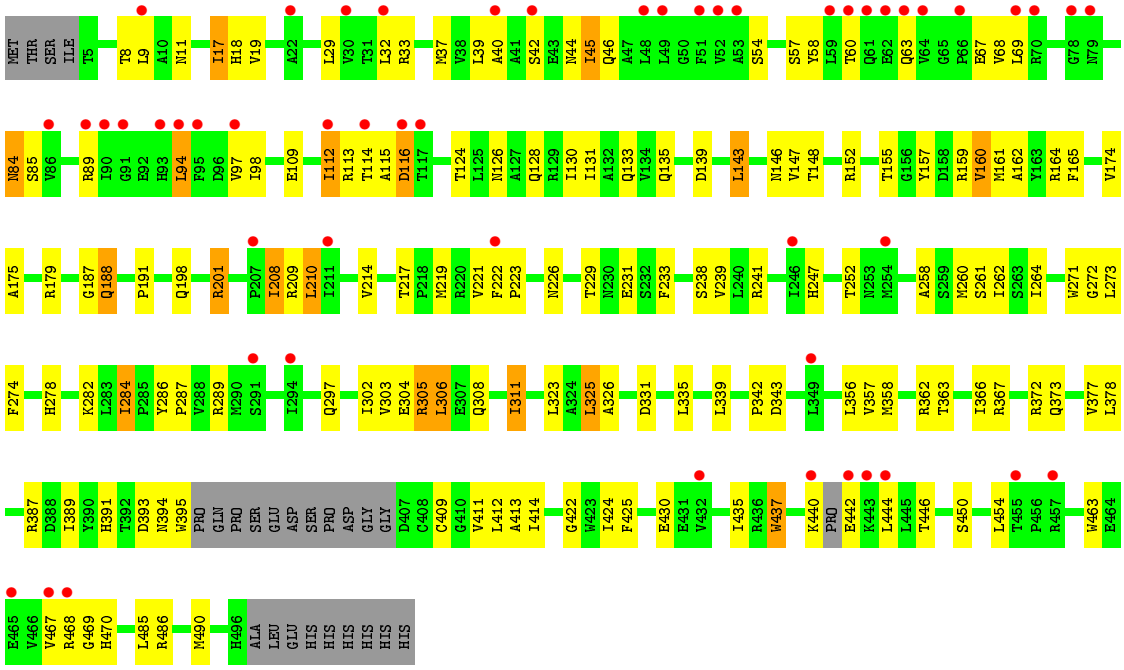
- Molecule 1: Bacteriophytochrome

Chain C:



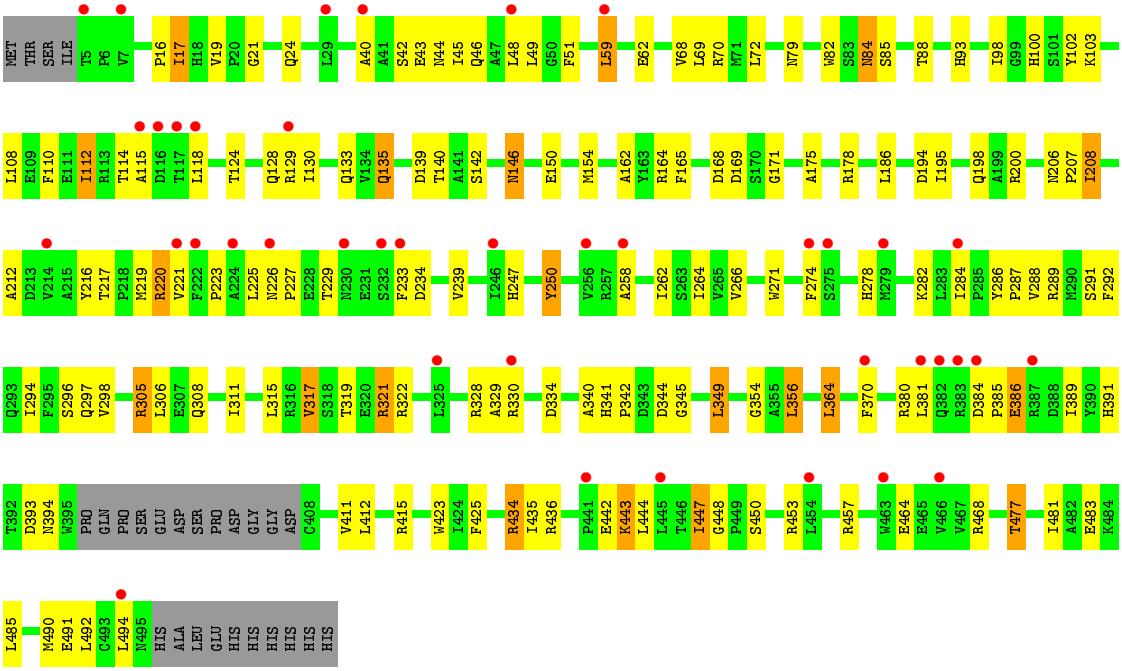
- Molecule 1: Bacteriophytochrome

Chain D:



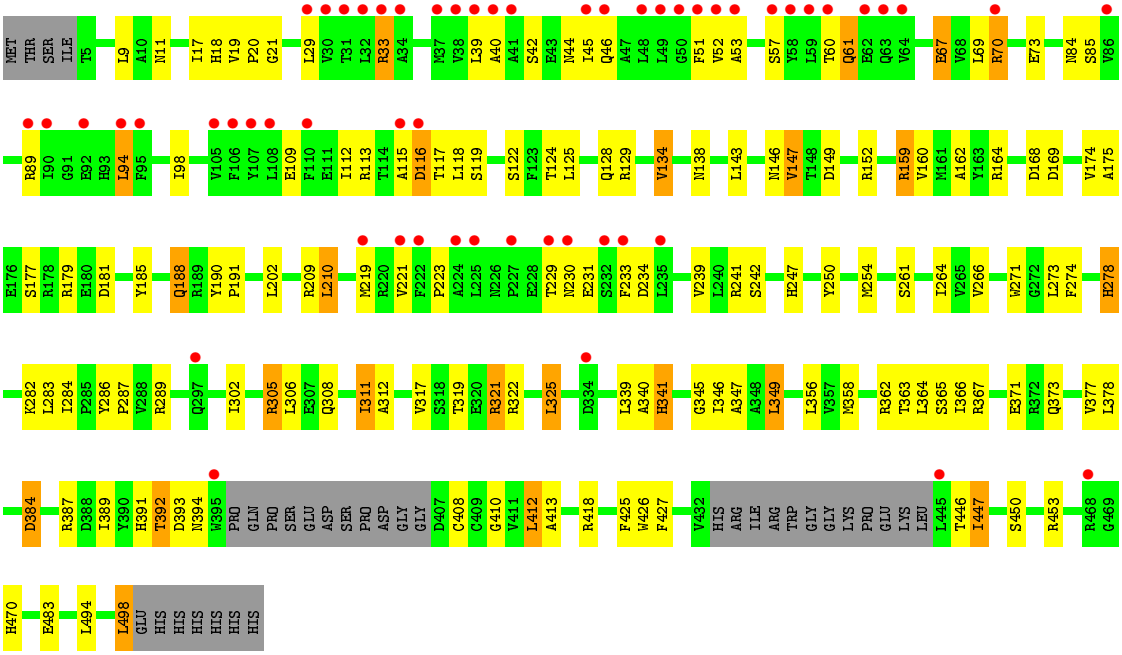
- Molecule 1: Bacteriophytochrome

Chain E:



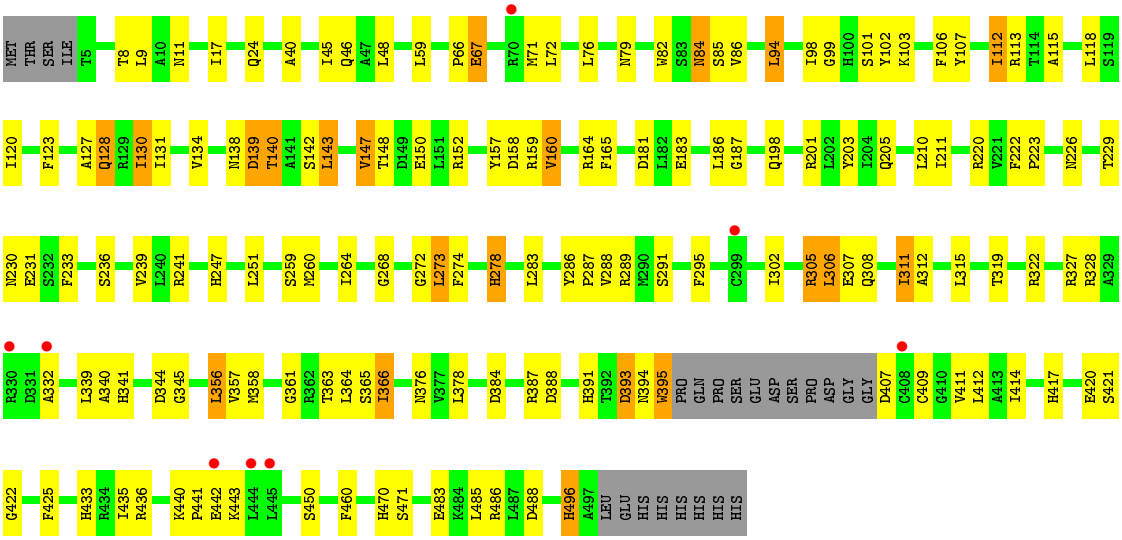
- Molecule 1: Bacteriophytochrome

Chain F:



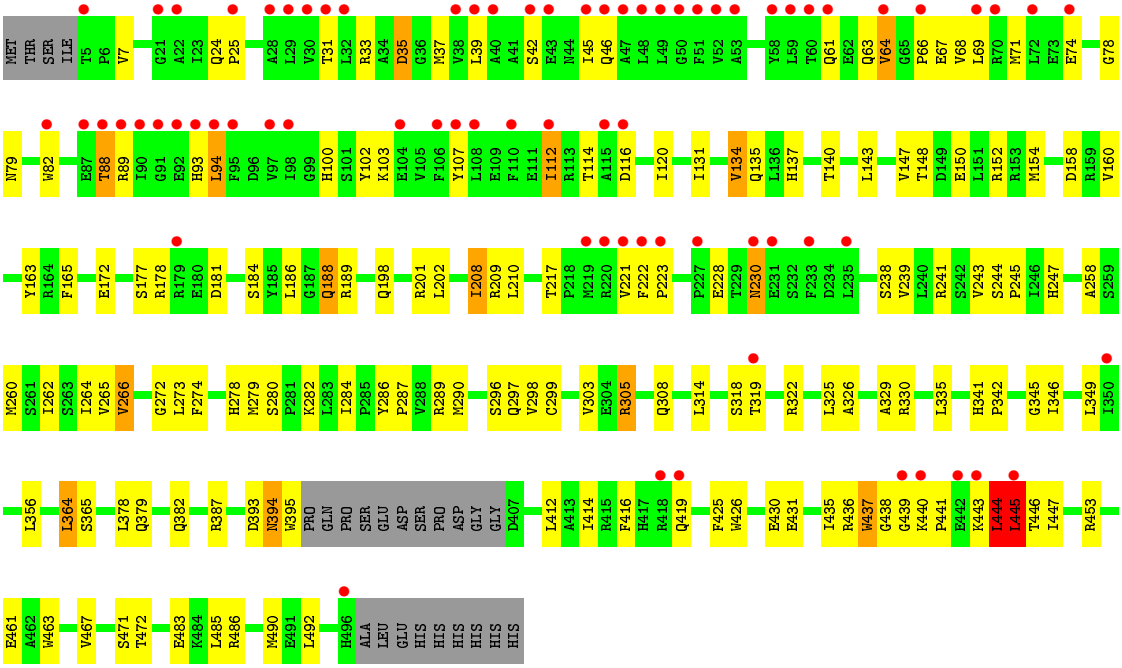
- Molecule 1: Bacteriophytochrome

Chain G:



- Molecule 1: Bacteriophytochrome

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	154.38Å 162.98Å 436.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.55 49.49 – 2.53	Depositor EDS
% Data completeness (in resolution range)	82.9 (48.48-2.55) 81.3 (49.49-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.215 , 0.258 0.216 , 0.256	Depositor DCC
R_{free} test set	7397 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 148657 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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 (i)

5.1 Standard geometry (i)

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

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	0.26	0/3874	0.48	0/5258
1	B	0.24	0/3789	0.45	0/5144
1	C	0.25	0/3897	0.46	0/5289
1	D	0.24	0/3884	0.45	0/5269
1	E	0.23	0/3874	0.45	0/5258
1	F	0.23	0/3797	0.45	0/5155
1	G	0.25	0/3904	0.47	0/5299
1	H	0.24	0/3893	0.44	0/5284
All	All	0.24	0/30912	0.46	0/41956

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	A	441	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	92	GLU	Peptide
1	C	62	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	3734	104	0
1	B	3709	0	3641	119	0
1	C	3812	0	3750	108	0
1	D	3801	0	3739	122	0
1	E	3790	0	3736	124	0
1	F	3717	0	3652	125	0
1	G	3816	0	3757	116	0
1	H	3808	0	3747	115	0
2	A	43	0	30	4	0
2	B	43	0	31	8	0
2	C	43	0	31	14	0
2	D	43	0	31	5	0
2	E	43	0	30	7	0
2	F	43	0	31	9	0
2	G	43	0	30	5	0
2	H	43	0	31	6	0
3	A	61	0	0	4	0
3	B	16	0	0	1	0
3	C	44	0	0	4	0
3	D	14	0	0	6	0
3	E	15	0	0	4	0
3	F	7	0	0	1	0
3	G	37	0	0	0	0
3	H	7	0	0	0	0
All	All	30788	0	30001	925	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 15.

All (925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:ARG:HG3	1:F:70:ARG:HH11	1.00	1.10
1:H:444:LEU:HD23	1:H:444:LEU:H	1.26	0.96
1:F:70:ARG:HG3	1:F:70:ARG:NH1	1.76	0.93
1:G:84:ASN:HD22	1:G:85:SER:H	1.02	0.92
1:D:112:ILE:HD13	1:D:112:ILE:H	1.36	0.91
1:A:364:LEU:HD21	1:G:435:ILE:HB	1.53	0.90
1:G:319:THR:HG22	1:G:322:ARG:HH21	1.36	0.89
1:C:41:ALA:HB1	1:C:45:ILE:HD12	1.53	0.89
1:E:447:ILE:HG12	1:E:448:GLY:N	1.87	0.88
1:C:17:ILE:HD11	3:C:909:HOH:O	1.75	0.87
1:A:140:THR:HG22	1:A:306:LEU:HB3	1.56	0.86
1:D:201:ARG:HG3	1:D:201:ARG:HH11	1.41	0.85
1:C:84:ASN:HD22	1:C:85:SER:H	1.24	0.85
1:B:7:VAL:HG21	1:B:245:PRO:HG2	1.57	0.84
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.41	0.84
1:G:394:ASN:HD21	1:G:470:HIS:CD2	1.95	0.84
2:C:900:BLA:HBC1	2:C:900:BLA:HMC1	1.58	0.84
1:G:198:GLN:HE22	1:G:201:ARG:NH1	1.75	0.83
1:H:441:PRO:HB3	1:H:443:LYS:HE2	1.61	0.82
1:G:84:ASN:HD22	1:G:85:SER:N	1.77	0.82
1:D:394:ASN:O	1:D:395:TRP:HB2	1.80	0.81
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.61	0.81
1:D:201:ARG:CG	1:D:201:ARG:HH11	1.93	0.81
1:D:139:ASP:HB3	3:D:910:HOH:O	1.81	0.81
1:E:17:ILE:HG22	3:E:909:HOH:O	1.80	0.81
1:G:120:ILE:HA	1:H:120:ILE:HD11	1.63	0.81
1:D:124:THR:HG22	3:D:909:HOH:O	1.80	0.80
1:H:33:ARG:HG2	1:H:37:MET:HB3	1.64	0.80
1:H:440:LYS:N	1:H:441:PRO:HD2	1.96	0.80
1:D:37:MET:HB2	1:D:58:TYR:CZ	2.19	0.78
1:F:210:LEU:HD12	1:F:289:ARG:HD3	1.65	0.78
1:E:305:ARG:HA	1:E:308:GLN:HG2	1.63	0.78
1:H:198:GLN:HE22	1:H:201:ARG:HH11	1.32	0.76
1:F:70:ARG:CG	1:F:70:ARG:HH11	1.91	0.76
1:H:198:GLN:NE2	1:H:201:ARG:HH11	1.83	0.75
1:A:479:LEU:O	1:A:483:GLU:HG3	1.86	0.75
1:F:356:LEU:HD23	1:F:365:SER:HB3	1.69	0.75
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.69	0.75
1:H:258:ALA:HB3	1:H:278:HIS:HB3	1.68	0.74
1:G:378:LEU:HD11	1:G:425:PHE:HZ	1.52	0.74
1:A:143:LEU:O	1:A:147:VAL:HG12	1.87	0.74
1:D:188:GLN:NE2	2:D:900:BLA:HBB1	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:VAL:HG12	1:H:266:VAL:O	1.89	0.73
1:C:41:ALA:HB1	1:C:45:ILE:CD1	2.17	0.73
1:B:139:ASP:HB2	1:B:142:SER:HB2	1.70	0.73
1:B:356:LEU:HD23	1:B:365:SER:HB3	1.71	0.73
1:A:117:THR:HG22	1:A:118:LEU:H	1.54	0.73
1:G:210:LEU:HD23	1:G:260:MET:HG2	1.70	0.72
1:B:258:ALA:HB3	1:B:278:HIS:HB3	1.72	0.72
1:B:214:VAL:HB	1:B:257:ARG:HA	1.69	0.72
1:H:230:ASN:HD22	1:H:230:ASN:N	1.88	0.72
1:G:139:ASP:HB2	1:G:142:SER:HB2	1.70	0.72
1:D:89:ARG:HA	1:D:94:LEU:HA	1.71	0.71
1:E:434:ARG:HD2	1:E:435:ILE:HG23	1.70	0.71
1:C:475:SER:HB2	1:C:478:ASP:H	1.55	0.71
1:F:447:ILE:H	1:F:447:ILE:HD13	1.55	0.71
1:H:346:ILE:O	1:H:426:TRP:HZ3	1.74	0.71
1:B:305:ARG:HA	1:B:308:GLN:HG2	1.73	0.71
1:E:84:ASN:HD22	1:E:85:SER:H	1.39	0.70
1:D:210:LEU:HD12	1:D:289:ARG:HD3	1.73	0.70
1:H:305:ARG:HD2	1:H:305:ARG:N	2.06	0.70
1:E:194:ASP:HB3	2:E:900:BLA:HHB	1.73	0.70
1:A:440:LYS:HD2	1:G:361:GLY:HA3	1.74	0.69
1:B:410:GLY:O	1:B:427:PHE:HA	1.92	0.69
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.27	0.69
1:H:444:LEU:HD23	1:H:444:LEU:N	2.05	0.69
1:E:140:THR:HG22	1:E:306:LEU:HB3	1.75	0.69
1:H:112:ILE:H	1:H:112:ILE:HD13	1.56	0.69
1:B:220:ARG:HE	1:B:222:PHE:HZ	1.41	0.69
1:E:88:THR:HG21	3:E:908:HOH:O	1.93	0.69
1:B:208:ILE:HD11	1:B:293:GLN:N	2.06	0.69
1:C:94:LEU:H	1:C:94:LEU:HD22	1.58	0.69
1:G:128:GLN:HA	1:H:297:GLN:HE22	1.55	0.69
1:G:127:ALA:O	1:G:131:ILE:HG23	1.93	0.69
1:E:317:VAL:O	1:E:321:ARG:HG2	1.93	0.69
1:F:305:ARG:HH11	1:F:305:ARG:HG2	1.58	0.69
1:E:305:ARG:HH21	1:E:308:GLN:HE22	1.41	0.68
1:G:131:ILE:HD11	1:H:297:GLN:HB3	1.75	0.68
1:H:286:TYR:HB3	1:H:287:PRO:HD3	1.75	0.68
1:E:328:ARG:HH12	1:E:344:ASP:HB2	1.57	0.68
1:E:297:GLN:HE22	1:F:128:GLN:HA	1.58	0.68
1:F:45:ILE:HD12	1:F:46:GLN:H	1.59	0.68
1:D:157:TYR:OH	1:D:284:ILE:HD11	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:HH21	1:B:376:ASN:HD21	1.42	0.67
1:C:84:ASN:ND2	1:C:85:SER:H	1.92	0.67
1:E:162:ALA:HB3	1:E:175:ALA:HB3	1.76	0.67
1:D:372:ARG:HB2	3:D:904:HOH:O	1.94	0.67
1:F:168:ASP:O	1:F:169:ASP:HB2	1.95	0.67
1:B:205:GLN:HE22	1:H:419:GLN:HG2	1.59	0.67
1:H:45:ILE:HD12	1:H:46:GLN:N	2.09	0.67
1:C:129:ARG:HE	1:C:154:MET:HG2	1.60	0.66
1:H:64:VAL:HG12	1:H:68:VAL:HG11	1.77	0.66
1:C:435:ILE:HD11	1:E:340:ALA:HB1	1.77	0.66
1:C:319:THR:HG22	1:C:322:ARG:HH21	1.58	0.66
1:A:444:LEU:HD22	1:A:444:LEU:H	1.60	0.66
1:C:17:ILE:HG12	3:C:930:HOH:O	1.94	0.66
1:G:157:TYR:HA	1:G:278:HIS:HD2	1.59	0.66
1:B:64:VAL:HG12	1:B:68:VAL:HB	1.78	0.66
1:F:239:VAL:HG11	1:F:289:ARG:HH21	1.60	0.66
1:D:356:LEU:HD21	1:D:363:THR:HG23	1.77	0.66
1:B:45:ILE:HD12	1:B:46:GLN:H	1.60	0.66
1:D:8:THR:H	1:D:11:ASN:HB3	1.60	0.65
1:E:464:GLU:O	1:E:468:ARG:HG2	1.97	0.65
1:E:442:GLU:HG3	1:E:443:LYS:H	1.62	0.65
1:H:89:ARG:HA	1:H:94:LEU:HA	1.79	0.65
1:C:328:ARG:HH12	1:C:344:ASP:HB2	1.61	0.65
1:A:9:LEU:HD21	1:A:450:SER:HB3	1.78	0.65
1:A:45:ILE:HD12	1:A:46:GLN:H	1.61	0.65
1:D:45:ILE:HD12	1:D:46:GLN:H	1.61	0.65
1:E:321:ARG:HH11	1:E:321:ARG:CG	2.09	0.65
1:C:148:THR:HG23	1:C:160:VAL:HG22	1.79	0.65
1:D:286:TYR:HB3	1:D:287:PRO:HD3	1.78	0.64
1:F:45:ILE:HD12	1:F:46:GLN:N	2.12	0.64
1:G:159:ARG:NH1	1:G:183:GLU:O	2.29	0.64
1:D:54:SER:OG	1:D:57:SER:HB3	1.97	0.64
1:E:381:LEU:O	1:E:381:LEU:HD13	1.97	0.64
1:B:9:LEU:HD22	1:B:9:LEU:H	1.62	0.64
1:G:143:LEU:O	1:G:147:VAL:HG13	1.98	0.64
1:F:346:ILE:HB	1:F:426:TRP:CH2	2.32	0.64
1:G:157:TYR:HA	1:G:278:HIS:CD2	2.33	0.64
1:B:201:ARG:HH21	1:B:236:SER:HB3	1.62	0.64
1:E:447:ILE:HG12	1:E:448:GLY:H	1.63	0.64
1:H:346:ILE:O	1:H:426:TRP:CZ3	2.51	0.63
1:D:435:ILE:HB	1:H:364:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ALA:HB1	1:E:492:LEU:HD21	1.79	0.63
1:F:179:ARG:NH1	1:F:181:ASP:HB3	2.14	0.63
1:F:319:THR:HG22	1:F:322:ARG:HH21	1.64	0.63
1:G:198:GLN:HE22	1:G:201:ARG:HH11	1.46	0.63
1:A:13:GLU:HG2	3:A:925:HOH:O	1.98	0.63
2:C:900:BLA:HMA2	2:C:900:BLA:O2A	1.99	0.62
1:G:198:GLN:NE2	1:G:201:ARG:NH1	2.47	0.62
1:B:308:GLN:O	1:B:311:ILE:HD13	1.99	0.62
1:A:226:ASN:HB3	1:A:229:THR:HG22	1.81	0.62
1:H:178:ARG:HE	1:H:184:SER:HB2	1.64	0.62
1:C:198:GLN:HE22	1:C:201:ARG:HE	1.46	0.62
1:F:317:VAL:O	1:F:321:ARG:HG2	1.99	0.62
1:F:46:GLN:HB2	1:F:52:VAL:HG22	1.80	0.62
1:G:220:ARG:HE	1:G:222:PHE:HZ	1.47	0.62
1:G:378:LEU:HD11	1:G:425:PHE:CZ	2.33	0.62
1:F:143:LEU:O	1:F:147:VAL:HG13	2.00	0.62
1:C:209:ARG:HD2	3:C:939:HOH:O	1.99	0.62
1:A:208:ILE:H	1:A:208:ILE:HD13	1.65	0.62
1:B:213:ASP:O	1:B:216:TYR:HB3	1.99	0.62
1:H:445:LEU:HD12	1:H:447:ILE:HG23	1.82	0.62
1:E:21:GLY:HA2	1:E:233:PHE:CE1	2.34	0.62
1:C:209:ARG:HH12	2:C:900:BLA:CGD	2.13	0.61
1:A:444:LEU:N	1:A:444:LEU:HD22	2.16	0.61
1:A:356:LEU:HD21	1:A:363:THR:HG23	1.83	0.61
1:C:165:PHE:CD1	1:C:272:GLY:HA2	2.36	0.61
1:G:140:THR:HG21	1:G:307:GLU:OE2	2.01	0.61
1:B:42:SER:O	1:B:45:ILE:HG13	2.00	0.61
1:F:152:ARG:HB2	1:F:160:VAL:HG11	1.83	0.61
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.64	0.61
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.66	0.61
1:A:229:THR:HG23	1:A:231:GLU:H	1.65	0.61
1:F:89:ARG:HG2	1:F:94:LEU:HB3	1.81	0.61
1:B:139:ASP:HB2	1:B:142:SER:CB	2.31	0.61
1:C:229:THR:HG23	1:C:231:GLU:H	1.64	0.60
1:H:319:THR:HG22	1:H:322:ARG:HH21	1.66	0.60
1:D:229:THR:HG23	1:D:231:GLU:H	1.66	0.60
1:D:258:ALA:HB3	1:D:278:HIS:HB3	1.83	0.60
1:G:327:ARG:HG2	1:H:330:ARG:NH2	2.16	0.60
1:G:143:LEU:C	1:G:143:LEU:HD12	2.22	0.60
1:B:130:ILE:HG23	1:B:154:MET:SD	2.42	0.60
1:B:51:PHE:HB2	1:B:63:GLN:OE1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:H	1:A:59:LEU:HD22	1.66	0.60
1:F:286:TYR:N	1:F:287:PRO:HD2	2.17	0.60
1:B:98:ILE:HG21	1:B:286:TYR:CD1	2.37	0.60
1:A:266:VAL:HG22	1:A:271:TRP:HB2	1.83	0.60
1:D:148:THR:HG23	1:D:160:VAL:HG22	1.83	0.60
1:D:201:ARG:CG	1:D:201:ARG:NH1	2.60	0.59
1:A:54:SER:O	1:A:57:SER:HB3	2.02	0.59
1:C:30:VAL:HG22	1:C:45:ILE:CD1	2.32	0.59
1:E:17:ILE:CD1	1:E:198:GLN:HB3	2.31	0.59
1:D:94:LEU:O	1:D:94:LEU:HD13	2.01	0.59
1:C:434:ARG:NH2	1:E:340:ALA:O	2.35	0.59
1:E:59:LEU:HD13	1:E:69:LEU:HD22	1.84	0.59
1:B:294:ILE:O	1:B:298:VAL:HG23	2.02	0.59
1:D:29:LEU:HD13	1:D:109:GLU:HG2	1.85	0.59
1:G:328:ARG:HH12	1:G:344:ASP:HB2	1.67	0.59
1:C:84:ASN:HD22	1:C:85:SER:N	1.95	0.59
1:B:349:LEU:HD12	1:B:481:ILE:HG21	1.84	0.59
1:A:486:ARG:O	1:A:490:MET:HG3	2.02	0.59
1:C:315:LEU:O	1:C:319:THR:HG23	2.02	0.59
2:C:900:BLA:HMB3	2:C:900:BLA:CMA	2.32	0.59
1:G:358:MET:O	1:G:422:GLY:HA2	2.02	0.59
1:E:84:ASN:ND2	1:E:85:SER:H	2.01	0.59
1:C:417:HIS:HD2	1:C:420:GLU:H	1.51	0.58
1:F:113:ARG:HH22	1:F:119:SER:HA	1.68	0.58
1:G:440:LYS:HG3	1:G:440:LYS:O	2.04	0.58
2:A:900:BLA:HMB3	2:A:900:BLA:CMA	2.33	0.58
1:F:188:GLN:NE2	2:F:900:BLA:OB	2.37	0.58
1:F:266:VAL:HG22	1:F:271:TRP:HB2	1.84	0.58
1:D:409:CYS:SG	1:D:430:GLU:HG3	2.43	0.58
1:G:98:ILE:HG21	1:G:286:TYR:CE1	2.38	0.58
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.01	0.58
1:E:24:GLN:HE22	1:E:212:ALA:H	1.51	0.58
1:C:134:VAL:HG12	1:C:302:ILE:HG12	1.84	0.58
1:H:158:ASP:OD2	1:H:279:MET:HG2	2.03	0.58
1:G:322:ARG:HD2	1:G:488:ASP:OD2	2.03	0.58
1:B:139:ASP:HB3	1:B:142:SER:H	1.68	0.58
1:F:373:GLN:O	1:F:377:VAL:HG23	2.04	0.58
1:F:346:ILE:O	1:F:426:TRP:HZ3	1.87	0.57
1:C:198:GLN:NE2	1:C:201:ARG:HE	2.01	0.57
1:F:264:ILE:HD11	1:F:274:PHE:CE1	2.39	0.57
1:A:366:ILE:O	1:A:367:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:NH2	1:G:340:ALA:O	2.37	0.57
1:B:140:THR:HA	1:B:306:LEU:HD23	1.84	0.57
1:B:8:THR:HG23	1:B:11:ASN:HB3	1.85	0.57
1:C:210:LEU:HD12	1:C:289:ARG:HD3	1.87	0.57
1:A:354:GLY:HA3	1:A:370:PHE:CE1	2.39	0.57
2:B:900:BLA:HMB3	2:B:900:BLA:CMA	2.34	0.57
1:G:134:VAL:HG13	1:G:302:ILE:HG21	1.85	0.57
1:G:123:PHE:CD2	1:H:120:ILE:HD12	2.39	0.57
1:H:230:ASN:HD22	1:H:230:ASN:H	1.53	0.57
1:E:21:GLY:HA2	1:E:233:PHE:CZ	2.39	0.57
1:A:148:THR:HG23	1:A:160:VAL:HG22	1.84	0.57
1:B:7:VAL:HG21	1:B:245:PRO:CG	2.33	0.57
1:H:444:LEU:CD2	1:H:444:LEU:H	2.05	0.57
1:B:112:ILE:HD13	1:B:112:ILE:H	1.67	0.57
1:F:152:ARG:HB2	1:F:160:VAL:CG1	2.35	0.57
1:G:264:ILE:HD11	1:G:274:PHE:CE1	2.39	0.57
1:G:72:LEU:O	1:G:76:LEU:HD13	2.05	0.57
1:G:139:ASP:HB2	1:G:142:SER:CB	2.35	0.57
1:B:137:HIS:NE2	1:B:146:ASN:ND2	2.52	0.57
1:C:366:ILE:O	1:C:367:ARG:HB2	2.05	0.57
1:H:45:ILE:HD12	1:H:46:GLN:H	1.69	0.57
1:D:187:GLY:HA3	1:D:435:ILE:HD11	1.87	0.57
1:E:239:VAL:HG11	1:E:289:ARG:NH2	2.19	0.57
1:E:45:ILE:HD12	1:E:46:GLN:N	2.19	0.57
1:F:113:ARG:HH21	1:F:287:PRO:HG3	1.70	0.56
1:B:102:TYR:CE2	1:B:103:LYS:HE2	2.41	0.56
1:A:130:ILE:HD11	1:A:150:GLU:HG2	1.87	0.56
1:H:114:THR:HG22	1:H:116:ASP:H	1.70	0.56
1:B:410:GLY:HA3	1:B:428:ARG:HB2	1.88	0.56
1:C:30:VAL:HG22	1:C:45:ILE:HD13	1.87	0.56
1:D:40:ALA:CB	1:D:223:PRO:HD2	2.34	0.56
1:B:179:ARG:HD2	1:B:181:ASP:OD2	2.06	0.56
1:F:308:GLN:HA	1:F:311:ILE:HD13	1.87	0.56
1:A:322:ARG:HD2	1:A:488:ASP:OD1	2.04	0.56
1:D:128:GLN:HB2	3:D:909:HOH:O	2.05	0.56
1:A:444:LEU:CD2	1:A:444:LEU:H	2.19	0.56
1:H:414:ILE:HD12	1:H:486:ARG:HB2	1.88	0.56
1:F:278:HIS:CD2	1:F:282:LYS:HD2	2.41	0.56
1:H:152:ARG:HB2	1:H:160:VAL:HG12	1.86	0.56
1:E:319:THR:HG22	1:E:322:ARG:HH21	1.71	0.56
1:D:67:GLU:H	1:D:67:GLU:CD	2.08	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:900:BLA:HMA2	2:E:900:BLA:O2A	2.06	0.56
1:B:408:CYS:SG	1:B:428:ARG:O	2.64	0.55
1:E:258:ALA:HB2	1:E:282:LYS:H	1.71	0.55
1:B:122:SER:HB3	1:B:125:LEU:HB2	1.87	0.55
1:C:194:ASP:OD2	1:C:453:ARG:NH2	2.38	0.55
1:D:40:ALA:HB2	1:D:223:PRO:HD2	1.88	0.55
1:F:340:ALA:HB2	1:F:364:LEU:HD21	1.89	0.55
1:F:384:ASP:OD2	1:F:387:ARG:HG3	2.06	0.55
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.17	0.55
1:G:8:THR:H	1:G:11:ASN:HB2	1.71	0.55
1:E:297:GLN:NE2	1:F:128:GLN:HA	2.21	0.55
1:H:439:GLY:C	1:H:441:PRO:HD2	2.26	0.55
2:C:900:BLA:CBC	2:C:900:BLA:HMC1	2.34	0.55
1:B:373:GLN:HE22	1:B:408:CYS:N	2.05	0.55
1:F:311:ILE:HG12	1:F:312:ALA:N	2.21	0.55
1:D:84:ASN:HD22	1:D:85:SER:H	1.55	0.55
1:E:250:TYR:HD2	2:E:900:BLA:OC	1.90	0.55
1:A:356:LEU:HD13	1:A:357:VAL:N	2.22	0.55
1:F:9:LEU:HD21	1:F:450:SER:HB2	1.88	0.55
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.42	0.55
1:E:164:ARG:O	1:E:171:GLY:HA2	2.07	0.55
1:D:394:ASN:O	1:D:395:TRP:CB	2.54	0.54
1:B:51:PHE:HB2	1:B:63:GLN:CD	2.27	0.54
1:B:137:HIS:CE1	1:B:146:ASN:HD22	2.25	0.54
1:F:188:GLN:HE21	2:F:900:BLA:HBB1	1.73	0.54
1:F:356:LEU:HB3	1:F:425:PHE:HB2	1.90	0.54
1:B:21:GLY:O	1:B:221:VAL:HG22	2.07	0.54
1:A:435:ILE:HB	1:G:364:LEU:HD11	1.88	0.54
1:G:339:LEU:HD12	1:G:357:VAL:HG11	1.90	0.54
1:A:305:ARG:HD2	1:B:306:LEU:HD13	1.88	0.54
1:F:418:ARG:N	1:F:418:ARG:HD2	2.22	0.54
2:B:900:BLA:O2A	2:B:900:BLA:HMA2	2.07	0.54
1:A:210:LEU:HD13	1:A:289:ARG:HD3	1.90	0.54
1:F:346:ILE:HG13	1:F:347:ALA:N	2.23	0.54
1:F:247:HIS:CD2	2:F:900:BLA:HBD1	2.43	0.54
1:B:16:PRO:O	1:B:20:PRO:HD3	2.08	0.54
1:B:340:ALA:HB2	1:B:364:LEU:HD21	1.89	0.54
1:C:185:TYR:O	1:C:188:GLN:HB2	2.08	0.54
2:H:900:BLA:CMA	2:H:900:BLA:HMB3	2.38	0.54
1:D:162:ALA:HB3	1:D:175:ALA:HB3	1.90	0.54
1:F:44:ASN:HB3	1:F:219:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:THR:HG23	1:F:231:GLU:H	1.73	0.54
1:D:114:THR:HG22	1:D:115:ALA:H	1.72	0.54
1:H:356:LEU:HB3	1:H:425:PHE:HB2	1.90	0.53
1:D:305:ARG:HE	1:D:308:GLN:NE2	2.07	0.53
1:H:379:GLN:O	1:H:382:GLN:HB2	2.09	0.53
1:C:54:SER:O	1:C:57:SER:HB3	2.08	0.53
1:C:435:ILE:HG23	1:E:364:LEU:HD21	1.89	0.53
1:B:19:VAL:N	1:B:20:PRO:CD	2.71	0.53
1:H:209:ARG:HH12	2:H:900:BLA:CGD	2.21	0.53
1:D:32:LEU:N	1:D:32:LEU:HD12	2.23	0.53
1:D:208:ILE:H	1:D:208:ILE:HD13	1.73	0.53
1:D:486:ARG:O	1:D:490:MET:HG3	2.08	0.53
1:E:45:ILE:O	1:E:49:LEU:HB2	2.08	0.53
1:G:341:HIS:O	1:G:345:GLY:HA3	2.08	0.53
1:G:376:ASN:HB3	1:G:395:TRP:HH2	1.74	0.53
1:F:321:ARG:HD3	1:F:349:LEU:HD22	1.91	0.53
1:B:134:VAL:CG1	1:B:302:ILE:HG12	2.39	0.53
1:A:164:ARG:HD2	3:A:952:HOH:O	2.08	0.53
1:B:152:ARG:HD2	1:B:177:SER:OG	2.09	0.53
1:D:271:TRP:CE2	1:D:303:VAL:HG11	2.44	0.53
1:F:51:PHE:N	1:F:51:PHE:CD2	2.75	0.53
1:A:42:SER:O	1:A:45:ILE:HG13	2.09	0.53
1:A:434:ARG:HG2	1:A:435:ILE:HG23	1.90	0.53
1:E:391:HIS:HA	1:E:411:VAL:O	2.09	0.53
1:E:415:ARG:HD3	1:E:423:TRP:CZ2	2.43	0.53
1:D:450:SER:CB	1:D:454:LEU:HD22	2.39	0.53
1:D:126:ASN:O	1:D:130:ILE:HG23	2.09	0.52
1:G:67:GLU:H	1:G:67:GLU:CD	2.11	0.52
1:C:33:ARG:HB3	1:C:39:LEU:HD11	1.90	0.52
1:G:273:LEU:C	1:G:273:LEU:HD12	2.30	0.52
1:B:205:GLN:NE2	1:H:419:GLN:HG2	2.21	0.52
1:D:356:LEU:HB3	1:D:425:PHE:HB2	1.90	0.52
1:E:385:PRO:O	1:E:386:GLU:HB2	2.09	0.52
1:B:356:LEU:HD21	1:B:363:THR:OG1	2.09	0.52
1:A:305:ARG:HA	1:A:308:GLN:HG2	1.91	0.52
1:H:152:ARG:HD3	1:H:177:SER:O	2.09	0.52
1:E:321:ARG:NH1	1:E:321:ARG:HG3	2.24	0.52
1:B:328:ARG:HB3	1:B:338:ALA:HB2	1.92	0.52
1:A:165:PHE:CD1	1:A:272:GLY:HA2	2.44	0.52
1:B:38:VAL:O	1:B:55:PRO:HA	2.10	0.52
1:F:356:LEU:HD21	1:F:363:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:CYS:SG	1:F:427:PHE:HB3	2.49	0.52
1:G:305:ARG:HA	1:G:308:GLN:HG2	1.92	0.52
1:H:286:TYR:O	1:H:290:MET:HG2	2.09	0.52
1:F:33:ARG:HB3	1:F:39:LEU:HD11	1.90	0.52
1:G:328:ARG:O	1:G:332:ALA:HB3	2.10	0.52
1:F:273:LEU:C	1:F:273:LEU:HD12	2.29	0.52
1:A:258:ALA:HB3	1:A:278:HIS:HB3	1.92	0.52
1:G:67:GLU:HB2	1:G:86:VAL:HG11	1.92	0.52
1:B:87:GLU:OE2	1:B:113:ARG:HG2	2.10	0.52
1:B:98:ILE:HG21	1:B:286:TYR:CE1	2.45	0.51
1:E:46:GLN:HA	1:E:49:LEU:O	2.10	0.51
1:B:134:VAL:HG13	1:B:302:ILE:HG12	1.92	0.51
1:F:61:GLN:HG2	1:F:69:LEU:CD1	2.40	0.51
2:H:900:BLA:HMA2	2:H:900:BLA:O2A	2.10	0.51
1:B:152:ARG:HB2	1:B:160:VAL:CG1	2.40	0.51
1:D:325:LEU:HD12	1:D:326:ALA:N	2.25	0.51
1:C:347:ALA:CB	1:C:366:ILE:HD11	2.40	0.51
1:H:209:ARG:HH11	1:H:209:ARG:HG2	1.76	0.51
1:F:29:LEU:HD13	1:F:109:GLU:HG2	1.92	0.51
1:G:229:THR:HG23	1:G:231:GLU:H	1.75	0.51
1:D:113:ARG:HG3	1:D:114:THR:O	2.10	0.51
1:E:48:LEU:HD11	1:E:93:HIS:CD2	2.45	0.51
1:F:134:VAL:HG22	1:F:302:ILE:HG21	1.92	0.51
1:F:98:ILE:HG21	1:F:286:TYR:CE1	2.46	0.51
1:B:286:TYR:N	1:B:287:PRO:HD2	2.26	0.51
1:G:152:ARG:HB2	1:G:160:VAL:CG1	2.40	0.51
1:E:354:GLY:HA3	1:E:370:PHE:CE1	2.45	0.51
1:C:464:GLU:O	1:C:468:ARG:HG2	2.10	0.51
1:E:43:GLU:OE1	1:E:220:ARG:HG3	2.10	0.51
1:H:208:ILE:H	1:H:208:ILE:HD13	1.76	0.51
1:F:19:VAL:N	1:F:20:PRO:HD3	2.24	0.51
1:C:45:ILE:HG23	1:C:49:LEU:HD12	1.92	0.51
1:H:258:ALA:HB2	1:H:282:LYS:H	1.76	0.51
1:B:46:GLN:HB2	1:B:52:VAL:HG22	1.93	0.51
1:F:209:ARG:NH1	2:F:900:BLA:O1D	2.43	0.51
1:D:44:ASN:HB2	1:D:219:MET:HG2	1.92	0.51
1:A:317:VAL:O	1:A:321:ARG:HB2	2.10	0.51
1:A:414:ILE:HG13	1:A:414:ILE:O	2.09	0.51
1:F:366:ILE:O	1:F:367:ARG:HB2	2.11	0.51
1:D:435:ILE:HB	1:H:364:LEU:CD1	2.40	0.51
1:H:202:LEU:HD13	1:H:241:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLN:HE22	1:C:211:ILE:HA	1.75	0.51
1:G:113:ARG:CZ	1:G:115:ALA:HB3	2.41	0.51
1:H:31:THR:HG22	1:H:107:TYR:CD1	2.46	0.51
1:E:68:VAL:HG23	3:E:908:HOH:O	2.10	0.51
1:E:42:SER:HA	1:E:221:VAL:HG12	1.93	0.51
1:H:325:LEU:O	1:H:325:LEU:HD13	2.11	0.51
1:A:364:LEU:HA	1:G:436:ARG:O	2.11	0.50
1:H:463:TRP:CZ2	1:H:467:VAL:HG11	2.47	0.50
1:F:61:GLN:HG2	1:F:69:LEU:HD11	1.93	0.50
1:F:250:TYR:O	1:F:254:MET:HG3	2.10	0.50
1:C:313:GLU:O	1:C:317:VAL:HG13	2.11	0.50
1:A:9:LEU:CD2	1:A:450:SER:HB3	2.42	0.50
1:H:445:LEU:HG	1:H:445:LEU:O	2.11	0.50
1:B:32:LEU:HD12	1:B:32:LEU:N	2.26	0.50
1:B:208:ILE:HD12	1:B:293:GLN:HB2	1.92	0.50
1:F:389:ILE:HD11	1:F:483:GLU:OE2	2.11	0.50
1:C:304:GLU:HG2	1:D:135:GLN:HE22	1.76	0.50
1:F:188:GLN:NE2	2:F:900:BLA:HBB1	2.25	0.50
1:B:21:GLY:O	1:B:221:VAL:HG13	2.12	0.50
1:F:17:ILE:O	1:F:241:ARG:HD2	2.11	0.50
1:G:319:THR:HG22	1:G:322:ARG:NH2	2.16	0.50
1:E:305:ARG:HH22	1:F:138:ASN:HD22	1.58	0.50
1:B:273:LEU:C	1:B:273:LEU:HD12	2.31	0.50
1:E:305:ARG:HA	1:E:308:GLN:CG	2.40	0.50
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.25	0.50
1:B:133:GLN:OE1	1:B:137:HIS:HE1	1.95	0.50
1:C:124:THR:O	1:C:128:GLN:HG3	2.12	0.50
1:C:155:THR:OG1	1:C:157:TYR:HD1	1.95	0.50
1:A:436:ARG:HH11	1:A:436:ARG:HG3	1.77	0.50
1:F:284:ILE:HG22	1:F:289:ARG:HG2	1.93	0.50
1:D:325:LEU:HD12	1:D:325:LEU:C	2.32	0.50
1:B:314:LEU:O	1:B:317:VAL:HG22	2.11	0.50
1:E:321:ARG:HH11	1:E:321:ARG:HG3	1.76	0.50
1:B:201:ARG:HH21	1:B:236:SER:CB	2.24	0.50
1:E:490:MET:O	1:E:494:LEU:HD23	2.12	0.50
1:H:230:ASN:ND2	1:H:230:ASN:N	2.58	0.49
1:D:155:THR:HB	1:D:157:TYR:HD1	1.76	0.49
1:A:308:GLN:O	1:A:311:ILE:HD13	2.11	0.49
1:F:308:GLN:HA	1:F:311:ILE:CD1	2.41	0.49
1:D:414:ILE:HD12	1:D:486:ARG:HB2	1.92	0.49
1:B:391:HIS:HA	1:B:411:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:440:LYS:N	1:H:441:PRO:CD	2.71	0.49
1:B:112:ILE:H	1:B:112:ILE:CD1	2.25	0.49
1:D:305:ARG:N	1:D:305:ARG:HD2	2.27	0.49
1:G:148:THR:HG23	1:G:160:VAL:HG22	1.94	0.49
1:B:54:SER:O	1:B:57:SER:HB3	2.12	0.49
1:F:239:VAL:HG11	1:F:289:ARG:NH2	2.26	0.49
1:E:330:ARG:HG2	1:E:492:LEU:HD11	1.94	0.49
1:F:164:ARG:HD2	1:F:174:VAL:HG11	1.94	0.49
1:D:19:VAL:HG12	1:D:233:PHE:O	2.12	0.49
1:D:366:ILE:O	1:D:367:ARG:HB2	2.13	0.49
1:E:262:ILE:CG2	1:E:296:SER:HB2	2.41	0.49
1:H:172:GLU:HB2	1:H:189:ARG:HD3	1.94	0.49
1:A:32:LEU:HD11	1:A:59:LEU:HD21	1.94	0.49
1:G:340:ALA:HB2	1:G:364:LEU:HD21	1.95	0.49
1:B:112:ILE:HD13	1:B:112:ILE:N	2.27	0.49
1:H:222:PHE:HA	1:H:223:PRO:C	2.33	0.49
1:B:88:THR:HG23	1:B:89:ARG:N	2.27	0.49
1:G:247:HIS:NE2	1:G:251:LEU:HD11	2.27	0.49
1:F:53:ALA:HB2	1:F:60:THR:HG21	1.93	0.49
1:H:71:MET:O	1:H:74:GLU:HG3	2.12	0.49
1:E:140:THR:CG2	1:E:306:LEU:HB3	2.42	0.49
1:H:150:GLU:O	1:H:154:MET:HG3	2.13	0.49
1:D:152:ARG:HH21	1:D:179:ARG:CG	2.26	0.49
1:C:418:ARG:HD2	1:G:205:GLN:HE22	1.78	0.49
2:F:900:BLA:CBC	2:F:900:BLA:HMC1	2.42	0.49
1:A:17:ILE:O	1:A:241:ARG:HD2	2.13	0.49
1:G:118:LEU:H	1:G:118:LEU:HD23	1.78	0.49
1:E:114:THR:HG22	1:E:115:ALA:N	2.27	0.49
1:D:373:GLN:O	1:D:377:VAL:HG23	2.13	0.49
1:B:24:GLN:HE22	1:B:211:ILE:HA	1.77	0.49
2:D:900:BLA:HBB1	2:D:900:BLA:OB	2.12	0.48
1:D:435:ILE:HA	1:H:365:SER:O	2.13	0.48
1:F:149:ASP:OD1	1:F:177:SER:HB3	2.13	0.48
1:H:394:ASN:O	1:H:395:TRP:HB2	2.13	0.48
1:D:33:ARG:HB3	1:D:39:LEU:CG	2.43	0.48
2:C:900:BLA:HBC1	2:C:900:BLA:CMC	2.38	0.48
2:G:900:BLA:HMB3	2:G:900:BLA:CMA	2.43	0.48
1:H:33:ARG:HB3	1:H:39:LEU:HD21	1.95	0.48
1:A:187:GLY:O	1:A:433:HIS:HE1	1.95	0.48
1:H:42:SER:HA	1:H:221:VAL:HA	1.95	0.48
1:C:139:ASP:HB3	1:C:142:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:HIS:O	1:F:392:THR:HG23	2.14	0.48
1:H:147:VAL:HG21	1:H:274:PHE:CZ	2.48	0.48
1:C:286:TYR:N	1:C:287:PRO:HD2	2.28	0.48
1:G:45:ILE:HD12	1:G:46:GLN:N	2.29	0.48
1:F:185:TYR:O	1:F:188:GLN:HB2	2.14	0.48
1:B:328:ARG:HH12	1:B:344:ASP:HB2	1.78	0.48
1:G:59:LEU:H	1:G:59:LEU:HD22	1.78	0.48
1:E:195:ILE:HG22	1:E:200:ARG:HB2	1.94	0.48
1:E:59:LEU:CD1	1:E:69:LEU:HD22	2.43	0.48
1:D:116:ASP:N	1:D:116:ASP:OD2	2.43	0.48
1:H:35:ASP:OD1	1:H:37:MET:HE3	2.13	0.48
1:D:98:ILE:HD12	1:D:239:VAL:HG21	1.95	0.48
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.79	0.48
1:F:116:ASP:N	1:F:117:THR:HB	2.29	0.48
1:C:365:SER:HB3	1:C:368:GLY:O	2.13	0.48
1:A:414:ILE:HD12	1:A:486:ARG:HB2	1.95	0.48
1:H:341:HIS:CG	1:H:342:PRO:HD2	2.48	0.48
1:A:286:TYR:N	1:A:287:PRO:HD2	2.29	0.48
1:D:18:HIS:ND1	1:D:198:GLN:HG2	2.29	0.48
1:D:247:HIS:CD2	2:D:900:BLA:HBD1	2.49	0.47
1:G:128:GLN:CA	1:H:297:GLN:HE22	2.25	0.47
2:F:900:BLA:HBC1	2:F:900:BLA:HMC1	1.95	0.47
1:G:134:VAL:CG1	1:G:302:ILE:HG12	2.44	0.47
1:F:325:LEU:C	1:F:325:LEU:HD12	2.34	0.47
1:D:155:THR:HB	1:D:157:TYR:CD1	2.49	0.47
1:C:284:ILE:HG22	1:C:289:ARG:HG2	1.96	0.47
1:C:323:LEU:HA	1:D:323:LEU:HD13	1.96	0.47
1:G:388:ASP:HB3	1:G:486:ARG:HE	1.78	0.47
1:F:283:LEU:C	1:F:284:ILE:HD12	2.34	0.47
1:A:42:SER:HA	1:A:221:VAL:HA	1.96	0.47
1:F:134:VAL:HG23	1:F:143:LEU:HD11	1.96	0.47
1:G:286:TYR:N	1:G:287:PRO:HD2	2.29	0.47
1:E:258:ALA:HB3	1:E:278:HIS:HB3	1.96	0.47
1:D:84:ASN:ND2	1:D:85:SER:H	2.12	0.47
1:E:48:LEU:HD23	1:E:112:ILE:HD12	1.95	0.47
1:H:238:SER:HB3	1:H:241:ARG:HB3	1.96	0.47
1:F:358:MET:SD	1:F:378:LEU:HD11	2.54	0.47
1:A:140:THR:CG2	1:A:306:LEU:HB3	2.36	0.47
1:H:364:LEU:HD12	1:H:364:LEU:C	2.34	0.47
2:F:900:BLA:HMB3	2:F:900:BLA:CMA	2.45	0.47
1:D:143:LEU:O	1:D:147:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:GLY:O	1:F:427:PHE:HA	2.15	0.47
1:B:208:ILE:HD11	1:B:292:PHE:C	2.35	0.47
1:G:158:ASP:H	1:G:278:HIS:CD2	2.33	0.47
1:H:94:LEU:HD13	1:H:94:LEU:O	2.15	0.47
1:F:19:VAL:HG12	1:F:234:ASP:HA	1.97	0.47
1:E:266:VAL:HG22	1:E:271:TRP:HB2	1.97	0.47
1:C:140:THR:HG21	1:C:307:GLU:OE2	2.14	0.47
1:E:286:TYR:HB3	1:E:287:PRO:HD3	1.96	0.47
1:G:150:GLU:OE1	1:G:150:GLU:HA	2.14	0.47
2:G:900:BLA:HBB1	2:G:900:BLA:OB	2.15	0.47
1:E:139:ASP:OD1	1:E:142:SER:HB2	2.14	0.47
1:B:299:CYS:O	1:B:303:VAL:HG23	2.14	0.47
1:E:44:ASN:HB3	1:E:219:MET:SD	2.55	0.47
1:B:130:ILE:O	1:B:133:GLN:HB2	2.14	0.47
1:B:95:PHE:CE2	1:B:112:ILE:HG22	2.50	0.47
1:H:188:GLN:HB3	1:H:188:GLN:HE21	1.59	0.47
1:A:70:ARG:O	1:A:74:GLU:HG2	2.15	0.47
2:D:900:BLA:HMB3	2:D:900:BLA:CMA	2.45	0.47
1:C:134:VAL:HG12	1:C:134:VAL:O	2.15	0.47
1:B:188:GLN:HG2	2:B:900:BLA:HBB1	1.97	0.47
1:E:84:ASN:HD22	1:E:85:SER:N	2.08	0.46
1:D:45:ILE:CD1	1:D:46:GLN:H	2.27	0.46
1:A:143:LEU:HD23	1:A:303:VAL:HG23	1.97	0.46
1:E:42:SER:CA	1:E:221:VAL:HG12	2.44	0.46
1:F:418:ARG:HD2	1:F:418:ARG:H	1.79	0.46
1:D:339:LEU:HD13	1:D:357:VAL:HG21	1.96	0.46
1:A:30:VAL:HG12	1:A:32:LEU:CD1	2.45	0.46
1:C:60:THR:H	1:C:63:GLN:HE21	1.63	0.46
1:H:314:LEU:O	1:H:318:SER:HB2	2.15	0.46
1:B:147:VAL:HG21	1:B:274:PHE:CZ	2.50	0.46
1:B:168:ASP:O	1:B:169:ASP:HB2	2.14	0.46
1:G:288:VAL:O	1:G:291:SER:HB3	2.15	0.46
1:F:363:THR:HG21	1:F:371:GLU:CD	2.36	0.46
1:G:356:LEU:HD13	1:G:357:VAL:N	2.31	0.46
1:C:94:LEU:HD13	1:C:94:LEU:N	2.31	0.46
1:A:417:HIS:CD2	1:A:420:GLU:H	2.33	0.46
1:F:394:ASN:HD21	1:F:470:HIS:CE1	2.33	0.46
1:E:250:TYR:CD2	2:E:900:BLA:OC	2.68	0.46
1:C:391:HIS:HA	1:C:411:VAL:O	2.15	0.46
1:B:209:ARG:NH1	2:B:900:BLA:O1D	2.47	0.46
1:B:19:VAL:H	1:B:20:PRO:CD	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ARG:HB2	1:E:380:ARG:NH1	2.31	0.46
1:H:165:PHE:CE1	1:H:272:GLY:HA2	2.51	0.46
1:F:42:SER:HA	1:F:221:VAL:HA	1.98	0.46
1:C:17:ILE:CD1	2:C:900:BLA:HMD1	2.45	0.46
2:C:900:BLA:HBB1	2:C:900:BLA:OB	2.16	0.46
1:C:152:ARG:HB2	1:C:160:VAL:CG1	2.46	0.46
1:F:261:SER:HA	1:F:274:PHE:O	2.16	0.46
1:E:258:ALA:HB2	1:E:282:LYS:N	2.31	0.46
1:A:278:HIS:CD2	1:A:282:LYS:HB2	2.51	0.46
2:G:900:BLA:HMA2	2:G:900:BLA:HBA2	1.97	0.46
1:F:115:ALA:C	1:F:117:THR:HB	2.36	0.46
1:A:159:ARG:HD3	1:A:161:MET:SD	2.56	0.46
1:D:209:ARG:O	1:D:260:MET:HA	2.16	0.46
1:H:186:LEU:HB2	1:H:437:TRP:HZ3	1.81	0.46
2:B:900:BLA:HMB3	2:B:900:BLA:HMA1	1.98	0.46
1:G:302:ILE:HA	1:G:305:ARG:HG2	1.98	0.46
1:D:152:ARG:HH21	1:D:179:ARG:HG3	1.81	0.46
1:H:134:VAL:CG2	1:H:143:LEU:HD13	2.46	0.46
1:F:190:TYR:HB2	1:F:191:PRO:HD2	1.97	0.46
1:A:33:ARG:HB3	1:A:39:LEU:HG	1.98	0.46
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.80	0.45
1:G:496:HIS:ND1	1:G:496:HIS:C	2.69	0.45
1:B:71:MET:O	1:B:74:GLU:HG2	2.15	0.45
1:B:373:GLN:NE2	1:B:407:ASP:HA	2.31	0.45
1:A:290:MET:CE	1:B:128:GLN:HE22	2.30	0.45
1:H:239:VAL:CG1	1:H:289:ARG:HH22	2.29	0.45
1:B:31:THR:HG22	1:B:107:TYR:HD1	1.81	0.45
1:D:42:SER:O	1:D:45:ILE:HG13	2.17	0.45
1:H:445:LEU:CD1	1:H:447:ILE:HG23	2.45	0.45
1:E:221:VAL:HG23	1:E:233:PHE:CZ	2.51	0.45
1:C:264:ILE:HD11	1:C:274:PHE:CE1	2.52	0.45
1:E:315:LEU:O	1:E:319:THR:HG23	2.17	0.45
1:D:389:ILE:HG23	1:D:414:ILE:HG22	1.98	0.45
1:F:51:PHE:HD2	1:F:51:PHE:N	2.14	0.45
1:D:33:ARG:HB3	1:D:39:LEU:HG	1.98	0.45
1:G:417:HIS:CD2	1:G:420:GLU:H	2.34	0.45
1:G:48:LEU:HD11	1:G:112:ILE:HD11	1.97	0.45
1:C:284:ILE:HG22	1:C:289:ARG:CG	2.46	0.45
1:A:354:GLY:HA3	1:A:370:PHE:CZ	2.52	0.45
1:H:148:THR:HG23	1:H:160:VAL:HG13	1.98	0.45
1:G:24:GLN:HE22	1:G:211:ILE:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PHE:CD1	1:D:272:GLY:HA2	2.51	0.45
1:B:266:VAL:HG23	1:B:266:VAL:O	2.16	0.45
1:D:161:MET:O	1:D:274:PHE:HA	2.17	0.45
1:G:138:ASN:HA	1:H:305:ARG:HH22	1.82	0.45
1:D:98:ILE:HG21	1:D:286:TYR:CD1	2.51	0.45
1:C:264:ILE:HB	1:C:272:GLY:O	2.16	0.45
2:H:900:BLA:HBB1	2:H:900:BLA:OB	2.17	0.45
1:G:414:ILE:HD12	1:G:486:ARG:HB2	1.98	0.45
1:F:21:GLY:O	1:F:221:VAL:HG22	2.16	0.45
1:H:416:PHE:O	1:H:490:MET:HG2	2.16	0.45
1:F:284:ILE:HG22	1:F:289:ARG:CG	2.47	0.45
2:D:900:BLA:HMA2	2:D:900:BLA:O2A	2.16	0.45
1:E:59:LEU:HD22	1:E:72:LEU:CD2	2.47	0.45
1:C:283:LEU:C	1:C:284:ILE:HD12	2.36	0.45
1:G:203:TYR:OH	2:G:900:BLA:HAA1	2.16	0.45
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.52	0.45
1:C:415:ARG:HD3	1:C:423:TRP:CZ2	2.51	0.45
1:F:159:ARG:HD2	3:F:509:HOH:O	2.16	0.45
1:B:257:ARG:HG3	1:B:279:MET:O	2.17	0.45
1:E:85:SER:HB2	1:E:98:ILE:HG22	1.98	0.45
2:E:900:BLA:HBB1	2:E:900:BLA:OB	2.17	0.45
1:A:363:THR:HG22	3:A:954:HOH:O	2.17	0.45
1:E:264:ILE:HD11	1:E:274:PHE:CZ	2.52	0.45
1:D:302:ILE:HG22	1:D:306:LEU:HD22	1.98	0.45
1:D:133:GLN:HG3	1:D:146:ASN:HD21	1.81	0.45
1:C:440:LYS:HA	1:C:440:LYS:HD3	1.80	0.45
1:H:443:LYS:O	1:H:444:LEU:O	2.33	0.45
1:F:339:LEU:HD22	1:F:346:ILE:HG23	1.99	0.45
1:E:59:LEU:HD22	1:E:72:LEU:HD23	1.98	0.45
1:B:18:HIS:CD2	1:B:19:VAL:HG13	2.51	0.45
1:G:94:LEU:HD22	1:G:113:ARG:HB3	1.99	0.45
1:B:71:MET:SD	1:B:86:VAL:HG23	2.56	0.45
1:G:187:GLY:O	1:G:433:HIS:HE1	2.00	0.45
1:D:217:THR:HG23	1:D:217:THR:O	2.17	0.45
1:H:305:ARG:HE	1:H:308:GLN:NE2	2.14	0.45
1:A:440:LYS:H	1:A:440:LYS:HG3	1.56	0.45
1:C:435:ILE:CD1	1:E:340:ALA:HB1	2.46	0.45
1:G:308:GLN:O	1:G:311:ILE:HD13	2.17	0.45
1:E:45:ILE:HD12	1:E:46:GLN:H	1.81	0.45
1:D:308:GLN:O	1:D:311:ILE:HD13	2.16	0.45
1:G:417:HIS:O	1:G:421:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:O	1:A:382:GLN:HG2	2.16	0.45
1:D:467:VAL:O	1:D:470:HIS:HB2	2.17	0.45
1:E:321:ARG:NH1	1:E:321:ARG:CG	2.72	0.45
1:E:442:GLU:OE2	1:E:457:ARG:HD2	2.17	0.45
1:G:417:HIS:HD2	1:G:420:GLU:H	1.65	0.45
1:H:7:VAL:HG21	1:H:245:PRO:HG2	1.99	0.45
1:A:24:GLN:HE22	1:A:212:ALA:H	1.63	0.45
1:D:342:PRO:O	1:D:343:ASP:HB2	2.16	0.45
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.81	0.45
1:C:273:LEU:HD12	1:C:273:LEU:C	2.37	0.45
1:A:220:ARG:HE	1:A:222:PHE:HZ	1.64	0.45
1:G:226:ASN:HB2	1:G:233:PHE:CE1	2.52	0.45
1:H:326:ALA:HB1	1:H:330:ARG:HH12	1.82	0.44
1:F:494:LEU:O	1:F:498:LEU:HD12	2.16	0.44
2:A:900:BLA:HMB3	2:A:900:BLA:HMA2	1.99	0.44
1:G:76:LEU:HD12	1:G:106:PHE:CE2	2.53	0.44
1:A:17:ILE:HB	3:A:939:HOH:O	2.16	0.44
1:D:33:ARG:HB3	1:D:39:LEU:HD11	1.98	0.44
1:D:264:ILE:HD11	1:D:274:PHE:CZ	2.52	0.44
1:C:495:ASN:HD21	1:D:331:ASP:CG	2.21	0.44
1:E:294:ILE:O	1:E:298:VAL:HG23	2.17	0.44
1:C:372:ARG:HH12	1:C:406:GLY:HA2	1.81	0.44
1:A:190:TYR:HB2	1:A:191:PRO:HD2	1.99	0.44
1:F:118:LEU:HB2	1:F:122:SER:HB2	1.99	0.44
1:C:356:LEU:HB3	1:C:425:PHE:HB2	1.99	0.44
1:C:372:ARG:NH1	1:C:406:GLY:HA2	2.33	0.44
1:A:394:ASN:O	1:A:395:TRP:HB2	2.17	0.44
1:H:435:ILE:O	1:H:435:ILE:HG13	2.17	0.44
1:C:209:ARG:NH1	2:C:900:BLA:CGD	2.81	0.44
1:E:305:ARG:HB3	1:E:305:ARG:HE	1.54	0.44
1:E:305:ARG:HE	1:E:308:GLN:NE2	2.14	0.44
1:C:102:TYR:O	1:C:103:LYS:HB2	2.18	0.44
1:D:222:PHE:HA	1:D:223:PRO:C	2.38	0.44
1:D:164:ARG:HG3	1:D:174:VAL:HG11	1.99	0.44
1:B:326:ALA:HB1	1:B:330:ARG:NH1	2.32	0.44
1:D:391:HIS:HA	1:D:411:VAL:O	2.17	0.44
1:A:5:THR:HB	1:A:6:PRO:HD2	1.99	0.44
1:C:159:ARG:NH1	1:C:183:GLU:O	2.49	0.44
1:G:201:ARG:NH2	1:G:236:SER:OG	2.51	0.44
1:G:131:ILE:HD11	1:H:297:GLN:CB	2.47	0.44
1:A:435:ILE:HG22	1:G:366:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ALA:HB2	1:C:366:ILE:HD11	1.98	0.44
1:E:165:PHE:HA	1:E:171:GLY:HA2	2.00	0.44
1:G:165:PHE:CD1	1:G:272:GLY:HA2	2.53	0.44
1:G:82:TRP:H	1:G:101:SER:HB3	1.83	0.44
1:E:356:LEU:HB3	1:E:425:PHE:HB2	1.99	0.44
1:A:84:ASN:HB2	1:A:99:GLY:O	2.18	0.44
1:G:356:LEU:HD22	1:G:365:SER:HB2	1.99	0.44
1:G:358:MET:HG3	1:G:363:THR:HG22	2.00	0.44
1:C:417:HIS:CD2	1:C:420:GLU:H	2.32	0.44
1:B:237:TYR:HB2	3:B:513:HOH:O	2.18	0.44
1:E:82:TRP:O	1:E:100:HIS:HA	2.18	0.44
1:B:59:LEU:N	1:B:59:LEU:HD22	2.33	0.44
1:C:30:VAL:HG22	1:C:45:ILE:HD11	2.00	0.44
1:H:112:ILE:N	1:H:112:ILE:HD13	2.29	0.44
2:G:900:BLA:HBA2	2:G:900:BLA:CMA	2.48	0.44
1:H:326:ALA:HB1	1:H:330:ARG:NH1	2.33	0.44
1:H:172:GLU:HG3	1:H:189:ARG:HD3	2.00	0.44
1:H:131:ILE:HG21	1:H:298:VAL:HG21	2.00	0.44
2:F:900:BLA:OB	2:F:900:BLA:HBB1	2.17	0.43
1:D:162:ALA:O	1:D:174:VAL:HG22	2.17	0.43
1:F:366:ILE:HG22	1:F:367:ARG:HG3	1.99	0.43
1:G:393:ASP:C	1:G:394:ASN:HD22	2.21	0.43
1:F:425:PHE:HB3	1:F:427:PHE:CE1	2.53	0.43
1:F:278:HIS:HD2	1:F:282:LYS:HB2	1.82	0.43
1:E:262:ILE:HG22	1:E:296:SER:HB2	2.00	0.43
1:E:169:ASP:HB3	1:E:200:ARG:CZ	2.48	0.43
1:A:214:VAL:HB	1:A:257:ARG:HA	2.00	0.43
1:E:311:ILE:HG23	1:E:477:THR:CG2	2.48	0.43
1:D:130:ILE:HG13	1:D:131:ILE:N	2.34	0.43
1:H:341:HIS:ND1	1:H:342:PRO:HD2	2.34	0.43
1:A:328:ARG:NH1	1:A:341:HIS:CD2	2.86	0.43
1:H:262:ILE:HG22	1:H:296:SER:HB3	2.00	0.43
1:D:238:SER:HB3	1:D:241:ARG:HB2	1.99	0.43
1:G:384:ASP:CG	1:G:387:ARG:HG3	2.39	0.43
1:E:208:ILE:HD13	1:E:208:ILE:H	1.82	0.43
1:F:67:GLU:H	1:F:67:GLU:CD	2.22	0.43
1:F:284:ILE:CG2	1:F:289:ARG:HG2	2.48	0.43
1:D:284:ILE:HB	1:D:289:ARG:HG3	2.00	0.43
1:B:201:ARG:CG	1:B:201:ARG:NH1	2.81	0.43
1:A:356:LEU:HD13	1:A:356:LEU:C	2.38	0.43
1:B:8:THR:CG2	1:B:11:ASN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LEU:HB3	1:E:51:PHE:CE2	2.53	0.43
1:H:264:ILE:HD11	1:H:274:PHE:CZ	2.53	0.43
1:B:31:THR:HG22	1:B:107:TYR:CD1	2.54	0.43
1:A:377:VAL:HG22	1:A:395:TRP:CH2	2.54	0.43
1:C:44:ASN:CG	1:C:219:MET:HG2	2.39	0.43
1:C:84:ASN:ND2	1:C:85:SER:N	2.62	0.43
1:H:356:LEU:HD13	1:H:356:LEU:C	2.38	0.43
1:B:323:LEU:C	1:B:323:LEU:HD23	2.39	0.43
1:C:17:ILE:HD12	2:C:900:BLA:HMD1	1.99	0.43
1:C:467:VAL:O	1:C:470:HIS:HB2	2.17	0.43
1:G:40:ALA:HB2	1:G:223:PRO:HD2	2.01	0.43
1:E:217:THR:O	1:E:217:THR:HG23	2.18	0.43
1:C:17:ILE:HD12	2:C:900:BLA:CMD	2.48	0.43
1:G:356:LEU:HB3	1:G:425:PHE:HB2	2.00	0.43
1:F:447:ILE:H	1:F:447:ILE:CD1	2.29	0.43
1:F:45:ILE:H	1:F:45:ILE:HG13	1.60	0.43
2:B:900:BLA:OB	2:B:900:BLA:HBB1	2.18	0.43
1:D:387:ARG:HB3	3:D:913:HOH:O	2.17	0.43
1:E:341:HIS:O	1:E:345:GLY:HA3	2.19	0.43
1:H:430:GLU:HA	1:H:471:SER:HA	2.00	0.43
1:D:437:TRP:HA	1:D:437:TRP:CE3	2.54	0.43
1:C:209:ARG:NH1	2:C:900:BLA:O1D	2.45	0.43
1:E:17:ILE:HD12	1:E:198:GLN:HB3	2.01	0.43
1:F:305:ARG:CG	1:F:305:ARG:HH11	2.28	0.43
1:B:188:GLN:HG2	2:B:900:BLA:CBB	2.49	0.43
1:H:165:PHE:CD1	1:H:272:GLY:HA2	2.53	0.43
1:B:229:THR:HG23	1:B:231:GLU:H	1.82	0.43
1:A:72:LEU:HD13	1:A:76:LEU:HD13	2.01	0.43
1:B:206:ASN:HA	1:B:207:PRO:HD2	1.87	0.43
1:D:191:PRO:HD3	1:D:463:TRP:HB2	2.00	0.43
1:B:261:SER:HA	1:B:274:PHE:O	2.19	0.43
1:D:467:VAL:HG23	1:D:468:ARG:N	2.34	0.43
1:H:260:MET:HE2	1:H:284:ILE:HD13	2.01	0.43
1:H:102:TYR:CZ	1:H:103:LYS:HE3	2.54	0.43
1:B:373:GLN:HE22	1:B:408:CYS:H	1.66	0.43
1:H:184:SER:HB3	1:H:437:TRP:CH2	2.54	0.43
1:B:51:PHE:CD2	1:B:51:PHE:N	2.87	0.43
1:A:247:HIS:CD2	2:A:900:BLA:HBD1	2.53	0.43
1:B:341:HIS:O	1:B:345:GLY:HA3	2.19	0.43
1:A:157:TYR:CD2	1:A:278:HIS:HB2	2.53	0.43
1:E:384:ASP:N	1:E:385:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LEU:HD12	1:E:48:LEU:HA	1.76	0.43
1:A:358:MET:O	1:A:422:GLY:HA2	2.19	0.43
1:E:389:ILE:HD11	1:E:483:GLU:OE2	2.19	0.43
1:G:84:ASN:ND2	1:G:85:SER:H	1.87	0.42
1:E:135:GLN:OE1	1:F:305:ARG:NH1	2.51	0.42
1:H:152:ARG:HB2	1:H:160:VAL:CG1	2.48	0.42
1:F:117:THR:HG23	1:F:117:THR:O	2.19	0.42
1:C:192:ALA:HA	3:C:938:HOH:O	2.17	0.42
3:D:906:HOH:O	1:H:436:ARG:HG3	2.19	0.42
1:D:273:LEU:HD12	1:D:273:LEU:C	2.39	0.42
1:D:9:LEU:HD22	1:D:9:LEU:H	1.83	0.42
1:H:78:GLY:HA2	1:H:79:ASN:HA	1.69	0.42
1:B:356:LEU:HD13	1:B:357:VAL:N	2.34	0.42
1:G:306:LEU:HD11	1:H:305:ARG:NH2	2.34	0.42
1:H:247:HIS:CD2	2:H:900:BLA:HBD1	2.54	0.42
1:A:391:HIS:HA	1:A:411:VAL:O	2.19	0.42
1:A:389:ILE:HD13	1:A:483:GLU:HG2	2.01	0.42
1:G:66:PRO:HG2	1:G:67:GLU:OE1	2.19	0.42
1:G:17:ILE:O	1:G:241:ARG:HD2	2.18	0.42
1:G:130:ILE:HG23	1:G:295:PHE:CD1	2.54	0.42
1:A:206:ASN:HA	1:A:207:PRO:HD2	1.80	0.42
1:B:13:GLU:H	1:B:13:GLU:HG3	1.70	0.42
1:C:389:ILE:HD11	1:C:483:GLU:HG2	2.01	0.42
1:C:295:PHE:HA	1:C:298:VAL:HG12	2.01	0.42
1:D:98:ILE:HG13	1:D:98:ILE:O	2.19	0.42
1:F:19:VAL:HG12	1:F:233:PHE:O	2.20	0.42
1:D:39:LEU:HD13	1:D:226:ASN:OD1	2.19	0.42
1:D:261:SER:HA	1:D:274:PHE:O	2.19	0.42
1:D:468:ARG:HG3	1:D:469:GLY:H	1.85	0.42
1:A:29:LEU:HD13	1:A:109:GLU:HG2	2.02	0.42
1:C:305:ARG:HD2	1:C:305:ARG:HA	1.92	0.42
1:D:393:ASP:N	1:D:393:ASP:OD2	2.53	0.42
1:E:16:PRO:HB2	1:E:19:VAL:HG22	2.01	0.42
1:A:30:VAL:HG12	1:A:32:LEU:HD13	2.02	0.42
1:D:60:THR:OG1	1:D:63:GLN:HG3	2.19	0.42
1:E:108:LEU:HB3	1:E:110:PHE:CE1	2.55	0.42
1:C:339:LEU:HD12	1:C:357:VAL:HG11	2.01	0.42
1:H:299:CYS:O	1:H:303:VAL:HB	2.19	0.42
1:C:247:HIS:CD2	2:C:900:BLA:HBD1	2.54	0.42
1:D:165:PHE:CE1	1:D:272:GLY:HA2	2.55	0.42
1:B:318:SER:O	1:B:322:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:TYR:O	1:E:103:LYS:HB2	2.19	0.42
1:H:24:GLN:HA	1:H:25:PRO:HD3	1.89	0.42
1:G:99:GLY:HA2	1:G:107:TYR:O	2.20	0.42
1:E:381:LEU:C	1:E:381:LEU:HD13	2.40	0.42
1:F:412:LEU:HB3	1:F:426:TRP:CD1	2.55	0.42
1:F:384:ASP:CG	1:F:387:ARG:HG3	2.40	0.42
1:A:210:LEU:HD12	1:A:260:MET:HG2	2.01	0.42
1:G:384:ASP:OD2	1:G:387:ARG:HG3	2.19	0.42
1:H:243:VAL:HG12	1:H:244:SER:N	2.35	0.42
1:A:133:GLN:OE1	1:A:146:ASN:HB3	2.19	0.42
1:D:358:MET:CE	1:D:378:LEU:HD11	2.50	0.42
1:G:394:ASN:ND2	1:G:470:HIS:CD2	2.75	0.42
1:B:247:HIS:CD2	2:B:900:BLA:HBD1	2.55	0.42
1:E:284:ILE:HD12	1:E:284:ILE:N	2.35	0.42
1:E:436:ARG:HG3	3:E:914:HOH:O	2.18	0.42
1:D:155:THR:O	1:D:282:LYS:HE2	2.20	0.42
1:D:363:THR:HB	1:H:438:GLY:O	2.20	0.42
1:C:201:ARG:O	1:C:205:GLN:HG2	2.20	0.42
1:E:42:SER:C	1:E:44:ASN:H	2.23	0.42
1:F:85:SER:HB3	1:F:98:ILE:HG22	2.02	0.42
1:G:440:LYS:O	1:G:442:GLU:N	2.53	0.42
1:F:44:ASN:OD1	1:F:219:MET:HG2	2.19	0.42
1:F:162:ALA:HB3	1:F:175:ALA:HB3	2.01	0.42
1:C:131:ILE:HD11	1:D:297:GLN:HB2	2.02	0.42
1:C:30:VAL:HG12	1:C:32:LEU:CD1	2.50	0.42
1:H:278:HIS:HD2	1:H:280:SER:O	2.03	0.42
1:B:45:ILE:HG13	1:B:45:ILE:H	1.63	0.42
1:C:152:ARG:HB2	1:C:160:VAL:HG13	2.02	0.42
1:B:152:ARG:HB2	1:B:160:VAL:HG11	2.01	0.42
1:F:413:ALA:HB2	1:F:425:PHE:CE2	2.55	0.41
1:A:147:VAL:HG13	1:A:274:PHE:HE2	1.85	0.41
1:D:42:SER:HA	1:D:221:VAL:HA	2.02	0.41
1:A:356:LEU:HB3	1:A:425:PHE:HB2	2.01	0.41
1:A:36:GLY:HA2	1:A:76:LEU:HD21	2.01	0.41
1:D:358:MET:O	1:D:422:GLY:HA2	2.20	0.41
1:A:318:SER:O	1:A:322:ARG:HG3	2.20	0.41
1:H:258:ALA:HB2	1:H:282:LYS:N	2.35	0.41
1:D:304:GLU:O	1:D:308:GLN:HG2	2.20	0.41
1:F:40:ALA:HB2	1:F:223:PRO:HD2	2.01	0.41
1:G:409:CYS:HB2	1:G:471:SER:HB3	2.01	0.41
1:B:408:CYS:SG	1:B:428:ARG:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:HA	1:F:94:LEU:HA	2.01	0.41
1:C:418:ARG:HH21	1:G:268:GLY:HA2	1.85	0.41
1:F:358:MET:CE	1:F:378:LEU:HD11	2.51	0.41
1:G:211:ILE:HB	1:G:259:SER:HB3	2.03	0.41
1:D:17:ILE:O	1:D:241:ARG:HD2	2.20	0.41
1:E:19:VAL:HG12	1:E:234:ASP:HA	2.02	0.41
1:D:358:MET:HE2	1:D:358:MET:HB3	1.75	0.41
1:D:214:VAL:HG11	1:D:252:THR:HG23	2.01	0.41
2:C:900:BLA:HMA2	2:C:900:BLA:HMB3	2.02	0.41
1:D:284:ILE:HD12	1:D:284:ILE:N	2.35	0.41
1:H:68:VAL:CG2	1:H:88:THR:HG21	2.50	0.41
1:A:444:LEU:C	1:A:445:LEU:O	2.58	0.41
1:F:152:ARG:HH21	1:F:179:ARG:HB3	1.85	0.41
1:H:186:LEU:HB2	1:H:437:TRP:CZ3	2.55	0.41
1:C:341:HIS:O	1:C:345:GLY:HA3	2.19	0.41
1:G:443:LYS:HD2	1:G:443:LYS:H	1.85	0.41
1:G:394:ASN:HD22	1:G:394:ASN:N	2.19	0.41
1:D:440:LYS:O	1:D:442:GLU:N	2.54	0.41
1:G:102:TYR:O	1:G:103:LYS:HB2	2.20	0.41
1:A:139:ASP:HB2	1:A:142:SER:OG	2.21	0.41
1:B:64:VAL:O	1:B:64:VAL:HG12	2.21	0.41
1:E:112:ILE:N	1:E:112:ILE:HD13	2.35	0.41
1:E:341:HIS:HA	1:E:342:PRO:HD3	1.84	0.41
1:G:239:VAL:HG11	1:G:289:ARG:NH2	2.35	0.41
1:A:491:GLU:HA	1:A:494:LEU:HD12	2.02	0.41
1:C:446:THR:HG23	1:C:446:THR:O	2.20	0.41
1:B:139:ASP:CB	1:B:142:SER:H	2.33	0.41
1:B:45:ILE:HD12	1:B:46:GLN:N	2.32	0.41
1:F:346:ILE:O	1:F:426:TRP:CZ3	2.70	0.41
1:E:284:ILE:O	1:E:289:ARG:HD3	2.21	0.41
1:F:18:HIS:CD2	1:F:19:VAL:HG13	2.56	0.41
1:F:341:HIS:O	1:F:345:GLY:HA3	2.21	0.41
1:H:82:TRP:O	1:H:100:HIS:HA	2.20	0.41
1:H:61:GLN:HA	1:H:69:LEU:HD11	2.02	0.41
1:B:329:ALA:HB3	1:B:492:LEU:HD21	2.03	0.41
1:C:147:VAL:HG21	1:C:274:PHE:CZ	2.56	0.41
1:B:349:LEU:HD12	1:B:481:ILE:CG2	2.50	0.41
2:A:900:BLA:HMA2	2:A:900:BLA:O2A	2.21	0.41
1:F:384:ASP:O	1:F:384:ASP:CG	2.59	0.41
1:F:164:ARG:HB2	1:F:174:VAL:CG1	2.50	0.41
1:C:374:ALA:O	1:C:378:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:THR:H	1:C:11:ASN:HB2	1.86	0.41
1:G:315:LEU:O	1:G:319:THR:HG23	2.21	0.41
1:B:208:ILE:HG12	1:B:262:ILE:CD1	2.51	0.41
1:F:147:VAL:CG2	1:F:274:PHE:CE2	3.04	0.41
1:C:261:SER:HA	1:C:274:PHE:O	2.20	0.41
1:F:202:LEU:HD13	1:F:241:ARG:CZ	2.50	0.41
1:A:152:ARG:NH2	1:A:179:ARG:HB3	2.36	0.41
1:C:42:SER:HA	1:C:221:VAL:HA	2.03	0.41
1:D:413:ALA:HA	1:D:424:ILE:O	2.21	0.41
1:E:130:ILE:HD11	1:E:150:GLU:HB2	2.02	0.41
1:C:7:VAL:O	1:C:7:VAL:HG23	2.21	0.41
1:C:288:VAL:O	1:C:291:SER:HB2	2.20	0.41
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.89	0.41
2:E:900:BLA:HMB3	2:E:900:BLA:CMA	2.51	0.41
1:A:69:LEU:O	1:A:73:GLU:HG3	2.20	0.41
1:G:9:LEU:HD21	1:G:450:SER:HB3	2.03	0.41
1:F:446:THR:HG23	1:F:446:THR:O	2.21	0.41
1:C:41:ALA:CB	1:C:45:ILE:HD12	2.38	0.40
1:H:42:SER:O	1:H:45:ILE:HG13	2.21	0.40
1:E:45:ILE:HG13	1:E:45:ILE:H	1.70	0.40
1:A:150:GLU:O	1:A:154:MET:HG3	2.20	0.40
1:G:433:HIS:CD2	1:G:460:PHE:CZ	3.09	0.40
1:E:311:ILE:HG23	1:E:477:THR:HG21	2.02	0.40
1:C:295:PHE:O	1:C:298:VAL:HG12	2.21	0.40
1:G:391:HIS:HA	1:G:411:VAL:O	2.20	0.40
1:C:435:ILE:HG23	1:E:364:LEU:CD2	2.51	0.40
1:F:339:LEU:HD22	1:F:346:ILE:CG2	2.50	0.40
1:F:9:LEU:HD22	1:F:9:LEU:H	1.86	0.40
1:A:243:VAL:HG12	1:A:244:SER:N	2.37	0.40
1:D:68:VAL:HG13	1:D:97:VAL:HG11	2.02	0.40
1:A:67:GLU:HB3	1:A:86:VAL:HG11	2.02	0.40
1:F:305:ARG:HG2	1:F:305:ARG:NH1	2.31	0.40
1:B:112:ILE:O	1:B:112:ILE:HG12	2.22	0.40
1:A:157:TYR:OH	1:A:260:MET:HB2	2.22	0.40
1:E:142:SER:O	1:E:146:ASN:HB2	2.21	0.40
1:E:291:SER:O	1:E:294:ILE:HB	2.21	0.40
1:E:294:ILE:HD11	1:F:124:THR:HA	2.03	0.40
1:B:226:ASN:O	1:B:230:ASN:N	2.55	0.40
1:E:129:ARG:O	1:E:133:GLN:HG2	2.21	0.40
1:C:19:VAL:O	1:C:19:VAL:HG23	2.21	0.40
1:E:305:ARG:HB3	1:E:308:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:HIS:CE1	2:E:900:BLA:CHA	3.04	0.40
1:D:362:ARG:HH12	1:H:178:ARG:NH2	2.19	0.40
1:G:71:MET:SD	1:G:86:VAL:HG23	2.62	0.40
1:E:168:ASP:O	1:E:169:ASP:HB2	2.21	0.40
1:G:414:ILE:HG13	1:G:414:ILE:O	2.20	0.40
1:A:33:ARG:HB3	1:A:39:LEU:CG	2.51	0.40
1:D:467:VAL:HG23	1:D:468:ARG:H	1.87	0.40
1:E:118:LEU:HA	1:E:118:LEU:HD23	1.88	0.40
1:E:349:LEU:HD22	1:E:481:ILE:HG21	2.04	0.40
1:E:206:ASN:HA	1:E:207:PRO:HD2	1.80	0.40
1:E:226:ASN:HA	1:E:227:PRO:HD3	1.94	0.40
1:C:475:SER:HB2	1:C:478:ASP:CG	2.42	0.40
1:D:356:LEU:C	1:D:356:LEU:HD13	2.41	0.40
1:F:89:ARG:HG2	1:F:94:LEU:CB	2.49	0.40
1:G:311:ILE:HD13	1:G:312:ALA:N	2.36	0.40
2:H:900:BLA:HMA1	2:H:900:BLA:HMB3	2.03	0.40
1:G:152:ARG:HB2	1:G:160:VAL:HG13	2.03	0.40
1:D:159:ARG:HD3	1:D:161:MET:HG3	2.04	0.40
1:E:118:LEU:HD12	1:E:288:VAL:HG13	2.03	0.40
1:E:288:VAL:HG12	1:E:292:PHE:CE2	2.57	0.40
1:E:40:ALA:HB2	1:E:223:PRO:HD2	2.04	0.40
1:H:329:ALA:HB1	1:H:492:LEU:HD21	2.02	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	475/505 (94%)	442 (93%)	30 (6%)	3 (1%)	30 48
1	B	464/505 (92%)	436 (94%)	28 (6%)	0	100 100
1	C	478/505 (95%)	455 (95%)	20 (4%)	3 (1%)	30 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	474/505 (94%)	451 (95%)	23 (5%)	0	100	100
1	E	475/505 (94%)	452 (95%)	22 (5%)	1 (0%)	52	73
1	F	465/505 (92%)	436 (94%)	27 (6%)	2 (0%)	39	60
1	G	479/505 (95%)	460 (96%)	18 (4%)	1 (0%)	52	73
1	H	477/505 (94%)	444 (93%)	28 (6%)	5 (1%)	19	33
All	All	3787/4040 (94%)	3576 (94%)	196 (5%)	15 (0%)	39	60

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	H	444	LEU
1	H	445	LEU
1	E	443	LYS
1	A	441	PRO
1	A	446	THR
1	C	62	GLU
1	C	81	PRO
1	H	345	GLY
1	F	242	SER
1	G	441	PRO
1	F	57	SER
1	C	66	PRO
1	H	66	PRO
1	H	266	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/431 (95%)	377 (92%)	31 (8%)	16	29
1	B	400/431 (93%)	365 (91%)	35 (9%)	12	22
1	C	410/431 (95%)	376 (92%)	34 (8%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	409/431 (95%)	384 (94%)	25 (6%)	23	40
1	E	408/431 (95%)	369 (90%)	39 (10%)	10	18
1	F	401/431 (93%)	366 (91%)	35 (9%)	13	22
1	G	411/431 (95%)	380 (92%)	31 (8%)	17	30
1	H	410/431 (95%)	370 (90%)	40 (10%)	10	17
All	All	3257/3448 (94%)	2987 (92%)	270 (8%)	14	25

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	GLU
1	A	32	LEU
1	A	45	ILE
1	A	69	LEU
1	A	89	ARG
1	A	108	LEU
1	A	120	ILE
1	A	135	GLN
1	A	140	THR
1	A	160	VAL
1	A	164	ARG
1	A	166	ARG
1	A	177	SER
1	A	186	LEU
1	A	208	ILE
1	A	217	THR
1	A	225	LEU
1	A	232	SER
1	A	239	VAL
1	A	250	TYR
1	A	283	LEU
1	A	311	ILE
1	A	327	ARG
1	A	380	ARG
1	A	387	ARG
1	A	412	LEU
1	A	440	LYS
1	A	443	LYS
1	A	453	ARG

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Mol	Chain	Res	Type
1	A	485	LEU
1	B	8	THR
1	B	11	ASN
1	B	13	GLU
1	B	32	LEU
1	B	45	ILE
1	B	61	GLN
1	B	70	ARG
1	B	76	LEU
1	B	88	THR
1	B	93	HIS
1	B	94	LEU
1	B	112	ILE
1	B	125	LEU
1	B	130	ILE
1	B	140	THR
1	B	178	ARG
1	B	180	GLU
1	B	181	ASP
1	B	198	GLN
1	B	201	ARG
1	B	210	LEU
1	B	250	TYR
1	B	257	ARG
1	B	273	LEU
1	B	291	SER
1	B	305	ARG
1	B	311	ILE
1	B	325	LEU
1	B	349	LEU
1	B	362	ARG
1	B	372	ARG
1	B	412	LEU
1	B	483	GLU
1	B	485	LEU
1	B	488	ASP
1	C	18	HIS
1	C	29	LEU
1	C	32	LEU
1	C	62	GLU
1	C	76	LEU
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	94	LEU
1	C	98	ILE
1	C	114	THR
1	C	117	THR
1	C	143	LEU
1	C	160	VAL
1	C	164	ARG
1	C	186	LEU
1	C	188	GLN
1	C	210	LEU
1	C	221	VAL
1	C	259	SER
1	C	260	MET
1	C	304	GLU
1	C	305	ARG
1	C	306	LEU
1	C	317	VAL
1	C	325	LEU
1	C	330	ARG
1	C	356	LEU
1	C	364	LEU
1	C	366	ILE
1	C	373	GLN
1	C	393	ASP
1	C	412	LEU
1	C	483	GLU
1	C	485	LEU
1	D	17	ILE
1	D	45	ILE
1	D	69	LEU
1	D	84	ASN
1	D	94	LEU
1	D	112	ILE
1	D	116	ASP
1	D	143	LEU
1	D	160	VAL
1	D	188	GLN
1	D	201	ARG
1	D	208	ILE
1	D	210	LEU
1	D	262	ILE

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Mol	Chain	Res	Type
1	D	284	ILE
1	D	305	ARG
1	D	306	LEU
1	D	311	ILE
1	D	325	LEU
1	D	335	LEU
1	D	412	LEU
1	D	437	TRP
1	D	444	LEU
1	D	446	THR
1	D	485	LEU
1	E	17	ILE
1	E	59	LEU
1	E	62	GLU
1	E	70	ARG
1	E	79	ASN
1	E	84	ASN
1	E	112	ILE
1	E	124	THR
1	E	128	GLN
1	E	135	GLN
1	E	146	ASN
1	E	154	MET
1	E	178	ARG
1	E	186	LEU
1	E	208	ILE
1	E	216	TYR
1	E	220	ARG
1	E	225	LEU
1	E	229	THR
1	E	250	TYR
1	E	305	ARG
1	E	317	VAL
1	E	321	ARG
1	E	334	ASP
1	E	349	LEU
1	E	356	LEU
1	E	364	LEU
1	E	386	GLU
1	E	393	ASP
1	E	394	ASN
1	E	412	LEU

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Mol	Chain	Res	Type
1	E	434	ARG
1	E	444	LEU
1	E	447	ILE
1	E	450	SER
1	E	453	ARG
1	E	477	THR
1	E	485	LEU
1	E	491	GLU
1	F	11	ASN
1	F	33	ARG
1	F	61	GLN
1	F	67	GLU
1	F	70	ARG
1	F	73	GLU
1	F	84	ASN
1	F	94	LEU
1	F	112	ILE
1	F	116	ASP
1	F	125	LEU
1	F	129	ARG
1	F	134	VAL
1	F	146	ASN
1	F	147	VAL
1	F	159	ARG
1	F	188	GLN
1	F	210	LEU
1	F	230	ASN
1	F	278	HIS
1	F	305	ARG
1	F	306	LEU
1	F	311	ILE
1	F	321	ARG
1	F	325	LEU
1	F	341	HIS
1	F	349	LEU
1	F	362	ARG
1	F	384	ASP
1	F	392	THR
1	F	393	ASP
1	F	412	LEU
1	F	447	ILE
1	F	453	ARG

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Mol	Chain	Res	Type
1	F	498	LEU
1	G	67	GLU
1	G	79	ASN
1	G	84	ASN
1	G	94	LEU
1	G	112	ILE
1	G	128	GLN
1	G	130	ILE
1	G	139	ASP
1	G	140	THR
1	G	143	LEU
1	G	147	VAL
1	G	160	VAL
1	G	164	ARG
1	G	181	ASP
1	G	186	LEU
1	G	230	ASN
1	G	273	LEU
1	G	278	HIS
1	G	283	LEU
1	G	305	ARG
1	G	306	LEU
1	G	311	ILE
1	G	356	LEU
1	G	366	ILE
1	G	393	ASP
1	G	395	TRP
1	G	407	ASP
1	G	412	LEU
1	G	483	GLU
1	G	485	LEU
1	G	496	HIS
1	H	35	ASP
1	H	63	GLN
1	H	64	VAL
1	H	67	GLU
1	H	88	THR
1	H	93	HIS
1	H	94	LEU
1	H	112	ILE
1	H	134	VAL
1	H	135	GLN

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Mol	Chain	Res	Type
1	H	137	HIS
1	H	140	THR
1	H	163	TYR
1	H	181	ASP
1	H	188	GLN
1	H	208	ILE
1	H	210	LEU
1	H	217	THR
1	H	228	GLU
1	H	230	ASN
1	H	273	LEU
1	H	305	ARG
1	H	335	LEU
1	H	349	LEU
1	H	364	LEU
1	H	378	LEU
1	H	387	ARG
1	H	393	ASP
1	H	394	ASN
1	H	412	LEU
1	H	431	GLU
1	H	437	TRP
1	H	444	LEU
1	H	445	LEU
1	H	446	THR
1	H	453	ARG
1	H	461	GLU
1	H	472	THR
1	H	483	GLU
1	H	485	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	128	GLN
1	A	198	GLN
1	A	230	ASN
1	A	293	GLN
1	A	391	HIS
1	A	394	ASN
1	A	417	HIS

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Mol	Chain	Res	Type
1	A	433	HIS
1	A	470	HIS
1	B	24	GLN
1	B	84	ASN
1	B	128	GLN
1	B	137	HIS
1	B	146	ASN
1	B	198	GLN
1	B	205	GLN
1	B	373	GLN
1	B	376	ASN
1	B	391	HIS
1	C	11	ASN
1	C	24	GLN
1	C	61	GLN
1	C	63	GLN
1	C	84	ASN
1	C	126	ASN
1	C	137	HIS
1	C	138	ASN
1	C	146	ASN
1	C	198	GLN
1	C	293	GLN
1	C	417	HIS
1	C	495	ASN
1	D	61	GLN
1	D	84	ASN
1	D	128	GLN
1	D	137	HIS
1	D	188	GLN
1	D	198	GLN
1	D	308	GLN
1	D	496	HIS
1	E	24	GLN
1	E	79	ASN
1	E	84	ASN
1	E	137	HIS
1	E	247	HIS
1	E	293	GLN
1	E	308	GLN
1	E	394	ASN
1	E	433	HIS

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Mol	Chain	Res	Type
1	F	24	GLN
1	F	26	HIS
1	F	84	ASN
1	F	128	GLN
1	F	133	GLN
1	F	138	ASN
1	F	198	GLN
1	F	247	HIS
1	F	293	GLN
1	F	394	ASN
1	F	417	HIS
1	G	24	GLN
1	G	84	ASN
1	G	128	GLN
1	G	146	ASN
1	G	198	GLN
1	G	205	GLN
1	G	278	HIS
1	G	293	GLN
1	G	394	ASN
1	G	417	HIS
1	G	419	GLN
1	G	433	HIS
1	G	470	HIS
1	H	24	GLN
1	H	46	GLN
1	H	93	HIS
1	H	126	ASN
1	H	133	GLN
1	H	188	GLN
1	H	198	GLN
1	H	230	ASN
1	H	247	HIS
1	H	297	GLN
1	H	308	GLN
1	H	373	GLN
1	H	433	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	BLA	A	900	1	35,46,46	2.80	14 (40%)	43,67,67	1.28	4 (9%)
2	BLA	B	900	1	35,46,46	2.89	14 (40%)	43,67,67	1.46	5 (11%)
2	BLA	C	900	1	35,46,46	2.81	16 (45%)	43,67,67	1.26	3 (6%)
2	BLA	D	900	1	35,46,46	2.86	14 (40%)	43,67,67	1.38	3 (6%)
2	BLA	E	900	1	35,46,46	2.91	14 (40%)	43,67,67	1.44	5 (11%)
2	BLA	F	900	1	35,46,46	2.80	13 (37%)	43,67,67	1.28	4 (9%)
2	BLA	G	900	1	35,46,46	2.86	13 (37%)	43,67,67	1.37	6 (13%)
2	BLA	H	900	1	35,46,46	2.83	13 (37%)	43,67,67	1.34	4 (9%)

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
2	BLA	A	900	1	-	1/22/74/74	0/4/4/4
2	BLA	B	900	1	-	1/22/74/74	0/4/4/4
2	BLA	C	900	1	-	1/22/74/74	0/4/4/4
2	BLA	D	900	1	-	1/22/74/74	0/4/4/4
2	BLA	E	900	1	-	1/22/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	F	900	1	-	1/22/74/74	0/4/4/4
2	BLA	G	900	1	-	1/22/74/74	0/4/4/4
2	BLA	H	900	1	-	1/22/74/74	0/4/4/4

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	C4D-C3D	-3.67	1.39	1.45
2	C	900	BLA	C4D-C3D	-3.58	1.39	1.45
2	G	900	BLA	C4D-C3D	-3.52	1.39	1.45
2	D	900	BLA	C4D-C3D	-3.51	1.39	1.45
2	H	900	BLA	C4D-C3D	-3.50	1.39	1.45
2	A	900	BLA	C4D-C3D	-3.49	1.39	1.45
2	A	900	BLA	C1D-C2D	-3.46	1.38	1.45
2	C	900	BLA	C1D-C2D	-3.45	1.38	1.45
2	E	900	BLA	C4D-C3D	-3.41	1.39	1.45
2	H	900	BLA	C1D-C2D	-3.40	1.38	1.45
2	F	900	BLA	C4D-C3D	-3.36	1.39	1.45
2	G	900	BLA	C1D-C2D	-3.33	1.38	1.45
2	F	900	BLA	C1C-C2C	-3.22	1.38	1.47
2	D	900	BLA	C1D-C2D	-3.20	1.38	1.45
2	F	900	BLA	C1D-C2D	-3.19	1.38	1.45
2	B	900	BLA	C1C-C2C	-3.18	1.38	1.47
2	C	900	BLA	C1B-C2B	-3.17	1.39	1.45
2	B	900	BLA	C1D-C2D	-3.17	1.38	1.45
2	G	900	BLA	C1C-C2C	-3.15	1.38	1.47
2	D	900	BLA	C3B-C4B	-3.15	1.37	1.47
2	C	900	BLA	C1C-C2C	-3.12	1.38	1.47
2	H	900	BLA	C1C-C2C	-3.10	1.38	1.47
2	E	900	BLA	C1D-C2D	-3.05	1.39	1.45
2	E	900	BLA	C3B-C4B	-3.04	1.38	1.47
2	D	900	BLA	C1C-C2C	-3.03	1.38	1.47
2	E	900	BLA	C1C-C2C	-3.02	1.38	1.47
2	B	900	BLA	CAB-C3B	-2.98	1.38	1.47
2	A	900	BLA	CAB-C3B	-2.97	1.38	1.47
2	E	900	BLA	CAB-C3B	-2.96	1.38	1.47
2	D	900	BLA	C1B-C2B	-2.94	1.39	1.45
2	H	900	BLA	C1B-C2B	-2.92	1.39	1.45
2	B	900	BLA	C1B-C2B	-2.91	1.39	1.45
2	D	900	BLA	CAB-C3B	-2.89	1.38	1.47
2	A	900	BLA	C1C-C2C	-2.87	1.39	1.47
2	G	900	BLA	C1B-C2B	-2.84	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	C1B-C2B	-2.83	1.39	1.45
2	H	900	BLA	C3B-C4B	-2.83	1.38	1.47
2	F	900	BLA	CAB-C3B	-2.82	1.39	1.47
2	A	900	BLA	C3B-C4B	-2.81	1.38	1.47
2	A	900	BLA	C1B-C2B	-2.79	1.39	1.45
2	G	900	BLA	C3B-C4B	-2.78	1.38	1.47
2	G	900	BLA	CAB-C3B	-2.77	1.39	1.47
2	H	900	BLA	CAB-C3B	-2.76	1.39	1.47
2	F	900	BLA	C1B-C2B	-2.73	1.39	1.45
2	C	900	BLA	CAB-C3B	-2.71	1.39	1.47
2	B	900	BLA	C3B-C4B	-2.69	1.39	1.47
2	C	900	BLA	C3B-C4B	-2.66	1.39	1.47
2	F	900	BLA	C3B-C4B	-2.37	1.40	1.47
2	E	900	BLA	C4C-NC	-2.14	1.34	1.37
2	A	900	BLA	C4C-NC	-2.14	1.34	1.37
2	C	900	BLA	C1C-NC	-2.09	1.33	1.37
2	A	900	BLA	C1B-NB	-2.08	1.34	1.37
2	C	900	BLA	C4C-NC	-2.08	1.34	1.37
2	B	900	BLA	C1B-NB	-2.07	1.34	1.37
2	G	900	BLA	C4C-NC	-2.05	1.34	1.37
2	F	900	BLA	C4C-NC	-2.05	1.34	1.37
2	E	900	BLA	C1B-NB	-2.04	1.34	1.37
2	C	900	BLA	C1B-NB	-2.04	1.34	1.37
2	H	900	BLA	C1B-NB	-2.03	1.34	1.37
2	B	900	BLA	C4C-NC	-2.02	1.34	1.37
2	D	900	BLA	C4C-NC	-2.00	1.34	1.37
2	D	900	BLA	CAC-C3C	2.14	1.54	1.47
2	C	900	BLA	CAC-C3C	2.15	1.54	1.47
2	C	900	BLA	C4A-CHB	3.04	1.51	1.40
2	A	900	BLA	C4A-CHB	3.14	1.52	1.40
2	F	900	BLA	C4A-CHB	3.17	1.52	1.40
2	H	900	BLA	C4A-CHB	3.32	1.52	1.40
2	G	900	BLA	C4A-CHB	3.32	1.52	1.40
2	B	900	BLA	C4A-CHB	3.34	1.53	1.40
2	D	900	BLA	C4A-CHB	3.35	1.53	1.40
2	E	900	BLA	C4A-CHB	3.42	1.53	1.40
2	C	900	BLA	CBC-CAC	4.64	1.53	1.30
2	F	900	BLA	CBC-CAC	4.67	1.53	1.30
2	F	900	BLA	CHA-C4D	4.67	1.39	1.35
2	E	900	BLA	CBC-CAC	4.69	1.53	1.30
2	B	900	BLA	CBC-CAC	4.69	1.53	1.30
2	A	900	BLA	CBC-CAC	4.70	1.53	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	BLA	CBC-CAC	4.71	1.53	1.30
2	H	900	BLA	CBC-CAC	4.71	1.53	1.30
2	D	900	BLA	CBC-CAC	4.74	1.53	1.30
2	C	900	BLA	CHD-C1D	4.84	1.52	1.40
2	H	900	BLA	CHD-C1D	4.86	1.52	1.40
2	A	900	BLA	CHD-C1D	4.90	1.52	1.40
2	D	900	BLA	CHA-C4D	5.01	1.39	1.35
2	C	900	BLA	CHA-C4D	5.04	1.39	1.35
2	A	900	BLA	CHA-C4D	5.11	1.39	1.35
2	H	900	BLA	CHA-C4D	5.13	1.39	1.35
2	B	900	BLA	CHD-C1D	5.26	1.53	1.40
2	G	900	BLA	CHD-C1D	5.28	1.53	1.40
2	D	900	BLA	CHD-C1D	5.28	1.53	1.40
2	F	900	BLA	CHD-C1D	5.30	1.53	1.40
2	G	900	BLA	CHA-C4D	5.31	1.39	1.35
2	E	900	BLA	CHD-C1D	5.33	1.53	1.40
2	B	900	BLA	CHA-C4D	5.34	1.39	1.35
2	E	900	BLA	CHA-C4D	5.57	1.40	1.35
2	A	900	BLA	CHD-C4C	5.97	1.52	1.37
2	C	900	BLA	CHD-C4C	6.14	1.52	1.37
2	H	900	BLA	CHD-C4C	6.23	1.52	1.37
2	G	900	BLA	CHD-C4C	6.39	1.53	1.37
2	D	900	BLA	CHD-C4C	6.39	1.53	1.37
2	F	900	BLA	CHD-C4C	6.45	1.53	1.37
2	E	900	BLA	CHD-C4C	6.55	1.53	1.37
2	B	900	BLA	CHD-C4C	6.60	1.53	1.37
2	C	900	BLA	CHB-C1B	7.85	1.52	1.34
2	D	900	BLA	CHB-C1B	8.03	1.52	1.34
2	F	900	BLA	CHB-C1B	8.04	1.52	1.34
2	A	900	BLA	CHB-C1B	8.06	1.52	1.34
2	B	900	BLA	CHB-C1B	8.20	1.52	1.34
2	H	900	BLA	CHB-C1B	8.20	1.52	1.34
2	G	900	BLA	CHB-C1B	8.20	1.52	1.34
2	E	900	BLA	CHB-C1B	8.24	1.52	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	BLA	C4C-CHD-C1D	-5.48	113.88	128.06
2	E	900	BLA	C4C-CHD-C1D	-5.33	114.28	128.06
2	D	900	BLA	C4C-CHD-C1D	-4.81	115.61	128.06
2	H	900	BLA	C4C-CHD-C1D	-4.40	116.67	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	900	BLA	C4C-CHD-C1D	-4.27	117.02	128.06
2	C	900	BLA	C4C-CHD-C1D	-3.80	118.23	128.06
2	F	900	BLA	C4C-CHD-C1D	-3.08	120.10	128.06
2	G	900	BLA	CBC-CAC-C3C	-3.07	111.45	127.01
2	B	900	BLA	CBC-CAC-C3C	-3.04	111.57	127.01
2	F	900	BLA	CBC-CAC-C3C	-3.01	111.76	127.01
2	H	900	BLA	CBC-CAC-C3C	-2.99	111.84	127.01
2	E	900	BLA	CBC-CAC-C3C	-2.94	112.07	127.01
2	A	900	BLA	CBC-CAC-C3C	-2.88	112.40	127.01
2	C	900	BLA	CBC-CAC-C3C	-2.60	113.80	127.01
2	D	900	BLA	CBC-CAC-C3C	-2.58	113.90	127.01
2	D	900	BLA	CHA-C4D-C3D	-2.50	119.68	125.55
2	C	900	BLA	CHA-C4D-C3D	-2.49	119.70	125.55
2	B	900	BLA	CHA-C4D-C3D	-2.49	119.70	125.55
2	F	900	BLA	CHA-C4D-C3D	-2.44	119.84	125.55
2	H	900	BLA	CHA-C4D-C3D	-2.43	119.86	125.55
2	G	900	BLA	CHA-C4D-C3D	-2.40	119.92	125.55
2	A	900	BLA	CHA-C4D-C3D	-2.30	120.16	125.55
2	E	900	BLA	CHA-C4D-C3D	-2.11	120.61	125.55
2	G	900	BLA	C4D-ND-C1D	2.01	110.48	106.51
2	H	900	BLA	CMB-C2B-C1B	2.02	126.89	124.20
2	A	900	BLA	CAD-C3D-C4D	2.04	128.70	125.06
2	G	900	BLA	CMB-C2B-C1B	2.05	126.92	124.20
2	B	900	BLA	C4D-ND-C1D	2.06	110.59	106.51
2	G	900	BLA	C1D-C2D-C3D	2.10	109.02	106.50
2	E	900	BLA	C4D-ND-C1D	2.12	110.70	106.51
2	A	900	BLA	CMB-C2B-C1B	2.19	127.11	124.20
2	B	900	BLA	CMB-C2B-C1B	2.20	127.13	124.20
2	F	900	BLA	CAD-C3D-C4D	2.39	129.33	125.06
2	E	900	BLA	CMB-C2B-C1B	2.69	127.78	124.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	900	BLA	C4A-CHB-C1B-NB
2	B	900	BLA	C4A-CHB-C1B-NB
2	D	900	BLA	C4A-CHB-C1B-NB
2	H	900	BLA	C4A-CHB-C1B-NB
2	E	900	BLA	C4A-CHB-C1B-NB
2	A	900	BLA	C4A-CHB-C1B-NB
2	C	900	BLA	C4A-CHB-C1B-NB

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Mol	Chain	Res	Type	Atoms
2	G	900	BLA	C4A-CHB-C1B-NB

There are no ring outliers.

8 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	4	0
2	B	900	BLA	8	0
2	C	900	BLA	14	0
2	D	900	BLA	5	0
2	E	900	BLA	7	0
2	F	900	BLA	9	0
2	G	900	BLA	5	0
2	H	900	BLA	6	0

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	479/505 (94%)	0.17	11 (2%) 64 69	37, 58, 109, 160	0
1	B	470/505 (93%)	0.74	54 (11%) 6 7	48, 88, 136, 183	0
1	C	482/505 (95%)	0.25	13 (2%) 58 63	39, 61, 102, 147	0
1	D	480/505 (95%)	0.71	52 (10%) 8 8	55, 92, 144, 191	0
1	E	479/505 (94%)	0.58	40 (8%) 14 15	49, 92, 134, 191	0
1	F	471/505 (93%)	0.66	56 (11%) 6 6	41, 81, 144, 171	0
1	G	482/505 (95%)	0.11	8 (1%) 73 77	37, 63, 105, 165	1 (0%)
1	H	481/505 (95%)	0.92	74 (15%) 3 3	55, 95, 158, 207	0
All	All	3824/4040 (94%)	0.52	308 (8%) 15 16	37, 79, 138, 207	1 (0%)

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	LEU	9.6
1	H	51	PHE	9.2
1	H	442	GLU	8.6
1	B	453	ARG	8.3
1	H	30	VAL	8.1
1	H	110	PHE	7.8
1	F	50	GLY	7.6
1	H	95	PHE	7.5
1	H	53	ALA	7.4
1	F	64	VAL	6.9
1	H	49	LEU	6.9
1	F	53	ALA	6.7
1	H	90	ILE	6.7
1	H	22	ALA	6.4
1	B	52	VAL	6.1
1	A	494	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	89	ARG	5.6
1	H	222	PHE	5.6
1	B	53	ALA	5.5
1	F	30	VAL	5.5
1	H	440	LYS	5.4
1	D	51	PHE	5.4
1	B	332	ALA	5.3
1	F	51	PHE	5.3
1	H	91	GLY	5.3
1	D	69	LEU	5.2
1	H	445	LEU	5.2
1	H	60	THR	5.2
1	B	51	PHE	5.2
1	D	59	LEU	5.1
1	F	32	LEU	5.1
1	A	445	LEU	5.0
1	D	90	ILE	5.0
1	D	53	ALA	5.0
1	H	58	TYR	5.0
1	B	69	LEU	4.8
1	H	223	PRO	4.8
1	H	32	LEU	4.7
1	H	230	ASN	4.7
1	B	58	TYR	4.6
1	B	59	LEU	4.6
1	F	63	GLN	4.6
1	F	225	LEU	4.6
1	H	45	ILE	4.6
1	B	224	ALA	4.6
1	H	28	ALA	4.5
1	H	231	GLU	4.5
1	A	90	ILE	4.5
1	E	214	VAL	4.5
1	F	222	PHE	4.5
1	B	331	ASP	4.4
1	H	227	PRO	4.4
1	B	468	ARG	4.4
1	H	29	LEU	4.3
1	H	52	VAL	4.3
1	B	62	GLU	4.3
1	F	49	LEU	4.3
1	D	116	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	494	LEU	4.2
1	E	454	LEU	4.2
1	F	89	ARG	4.2
1	D	30	VAL	4.1
1	A	93	HIS	4.1
1	F	90	ILE	4.1
1	E	48	LEU	4.1
1	A	330	ARG	4.1
1	D	49	LEU	4.1
1	G	444	LEU	4.0
1	D	66	PRO	4.0
1	H	89	ARG	4.0
1	D	443	LYS	3.9
1	E	330	ARG	3.9
1	H	39	LEU	3.8
1	B	496	HIS	3.8
1	D	95	PHE	3.8
1	B	222	PHE	3.8
1	H	64	VAL	3.8
1	B	9	LEU	3.8
1	F	105	VAL	3.7
1	B	55	PRO	3.7
1	F	29	LEU	3.7
1	D	52	VAL	3.7
1	D	64	VAL	3.7
1	B	93	HIS	3.7
1	F	45	ILE	3.7
1	E	230	ASN	3.7
1	E	221	VAL	3.6
1	E	494	LEU	3.6
1	B	338	ALA	3.6
1	D	444	LEU	3.6
1	H	233	PHE	3.6
1	C	442	GLU	3.6
1	E	384	ASP	3.6
1	A	329	ALA	3.6
1	B	37	MET	3.6
1	B	36	GLY	3.6
1	F	108	LEU	3.6
1	E	381	LEU	3.5
1	H	94	LEU	3.5
1	H	112	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	72	LEU	3.5
1	F	233	PHE	3.5
1	H	47	ALA	3.5
1	A	442	GLU	3.5
1	F	58	TYR	3.4
1	D	440	LYS	3.4
1	D	48	LEU	3.4
1	H	93	HIS	3.4
1	F	115	ALA	3.4
1	C	441	PRO	3.4
1	H	42	SER	3.4
1	B	446	THR	3.4
1	H	419	GLN	3.4
1	H	219	MET	3.4
1	D	32	LEU	3.3
1	F	221	VAL	3.3
1	D	114	THR	3.3
1	H	220	ARG	3.3
1	F	395	TRP	3.3
1	C	53	ALA	3.3
1	F	59	LEU	3.3
1	H	48	LEU	3.3
1	H	92	GLU	3.3
1	F	60	THR	3.3
1	C	439	GLY	3.3
1	F	110	PHE	3.3
1	F	116	ASP	3.2
1	F	95	PHE	3.2
1	D	62	GLU	3.2
1	D	9	LEU	3.2
1	E	59	LEU	3.2
1	C	444	LEU	3.2
1	F	39	LEU	3.2
1	H	61	GLN	3.2
1	H	115	ALA	3.2
1	E	383	ARG	3.1
1	F	334	ASP	3.1
1	H	21	GLY	3.1
1	D	432	VAL	3.1
1	F	33	ARG	3.1
1	E	224	ALA	3.1
1	D	40	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	104	GLU	3.1
1	E	117	THR	3.1
1	E	463	TRP	3.1
1	H	50	GLY	3.1
1	E	445	LEU	3.0
1	B	246	ILE	3.0
1	B	225	LEU	3.0
1	D	457	ARG	3.0
1	H	116	ASP	3.0
1	F	52	VAL	3.0
1	C	406	GLY	3.0
1	B	29	LEU	2.9
1	H	46	GLN	2.9
1	B	32	LEU	2.9
1	B	463	TRP	2.9
1	G	70	ARG	2.9
1	H	69	LEU	2.9
1	H	108	LEU	2.9
1	B	460	PHE	2.9
1	H	66	PRO	2.9
1	B	104	GLU	2.9
1	A	444	LEU	2.9
1	D	42	SER	2.9
1	D	91	GLY	2.9
1	E	7	VAL	2.9
1	F	235	LEU	2.9
1	B	447	ILE	2.9
1	D	61	GLN	2.9
1	D	467	VAL	2.8
1	F	224	ALA	2.8
1	E	116	ASP	2.8
1	G	445	LEU	2.7
1	D	112	ILE	2.7
1	B	235	LEU	2.7
1	F	92	GLU	2.7
1	B	48	LEU	2.7
1	B	333	ASP	2.7
1	D	207	PRO	2.7
1	H	5	THR	2.7
1	G	442	GLU	2.7
1	F	46	GLN	2.7
1	B	445	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	219	MET	2.6
1	H	97	VAL	2.6
1	H	82	TRP	2.6
1	H	235	LEU	2.6
1	B	5	THR	2.6
1	F	34	ALA	2.6
1	F	106	PHE	2.6
1	F	38	VAL	2.6
1	B	450	SER	2.6
1	E	258	ALA	2.6
1	F	40	ALA	2.6
1	D	93	HIS	2.6
1	F	86	VAL	2.6
1	D	222	PHE	2.6
1	F	468	ARG	2.5
1	E	274	PHE	2.5
1	D	291	SER	2.5
1	H	98	ILE	2.5
1	F	41	ALA	2.5
1	D	86	VAL	2.5
1	H	87	GLU	2.5
1	H	418	ARG	2.5
1	E	466	VAL	2.5
1	B	207	PRO	2.5
1	F	48	LEU	2.5
1	E	5	THR	2.5
1	C	335	LEU	2.4
1	D	117	THR	2.4
1	D	254	MET	2.4
1	E	222	PHE	2.4
1	G	299	CYS	2.4
1	F	70	ARG	2.4
1	C	128	GLN	2.4
1	D	79	ASN	2.4
1	D	63	GLN	2.4
1	H	31	THR	2.4
1	H	70	ARG	2.4
1	G	332	ALA	2.4
1	B	49	LEU	2.4
1	B	296	SER	2.4
1	D	294	ILE	2.4
1	H	439	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	246	ILE	2.3
1	D	468	ARG	2.3
1	F	297	GLN	2.3
1	F	232	SER	2.3
1	H	496	HIS	2.3
1	C	207	PRO	2.3
1	B	64	VAL	2.3
1	D	60	THR	2.3
1	D	89	ARG	2.3
1	E	382	GLN	2.3
1	F	107	TYR	2.3
1	D	97	VAL	2.3
1	E	40	ALA	2.3
1	E	29	LEU	2.3
1	F	230	ASN	2.3
1	E	256	VAL	2.3
1	F	229	THR	2.3
1	F	94	LEU	2.3
1	B	469	GLY	2.3
1	H	107	TYR	2.3
1	B	22	ALA	2.2
1	H	443	LYS	2.2
1	E	275	SER	2.2
1	B	334	ASP	2.2
1	B	343	ASP	2.2
1	E	233	PHE	2.2
1	H	74	GLU	2.2
1	H	319	THR	2.2
1	H	221	VAL	2.2
1	B	220	ARG	2.2
1	D	442	GLU	2.2
1	E	279	MET	2.2
1	F	62	GLU	2.2
1	D	22	ALA	2.2
1	H	40	ALA	2.2
1	B	208	ILE	2.2
1	E	118	LEU	2.2
1	F	31	THR	2.2
1	B	79	ASN	2.2
1	E	115	ALA	2.2
1	E	284	ILE	2.2
1	B	39	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	333	ASP	2.2
1	C	299	CYS	2.1
1	B	31	THR	2.1
1	E	441	PRO	2.1
1	F	37	MET	2.1
1	D	94	LEU	2.1
1	D	349	LEU	2.1
1	E	226	ASN	2.1
1	E	325	LEU	2.1
1	H	88	THR	2.1
1	H	43	GLU	2.1
1	F	227	PRO	2.1
1	D	78	GLY	2.1
1	D	70	ARG	2.1
1	B	203	TYR	2.1
1	D	211	ILE	2.1
1	A	48	LEU	2.1
1	E	387	ARG	2.1
1	H	25	PRO	2.1
1	G	408	CYS	2.1
1	E	370	PHE	2.1
1	F	445	LEU	2.1
1	D	465	GLU	2.1
1	F	57	SER	2.1
1	G	330	ARG	2.1
1	H	179	ARG	2.1
1	D	455	THR	2.1
1	E	129	ARG	2.0
1	E	246	ILE	2.0
1	H	350	ILE	2.0
1	B	299	CYS	2.0
1	H	38	VAL	2.0
1	B	63	GLN	2.0
1	B	294	ILE	2.0
1	B	366	ILE	2.0
1	E	232	SER	2.0
1	A	446	THR	2.0
1	B	237	TYR	2.0
1	C	295	PHE	2.0
1	H	106	PHE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	BLA	E	900	43/43	0.93	0.30	1.82	72,92,104,113	0
2	BLA	A	900	43/43	0.96	0.17	0.81	34,49,64,77	0
2	BLA	G	900	43/43	0.95	0.18	0.55	37,58,68,89	0
2	BLA	C	900	43/43	0.96	0.18	0.54	34,54,68,85	0
2	BLA	H	900	43/43	0.92	0.21	0.52	64,83,93,105	0
2	BLA	B	900	43/43	0.94	0.21	0.20	60,76,95,107	0
2	BLA	F	900	43/43	0.96	0.17	0.13	39,60,70,84	0
2	BLA	D	900	43/43	0.95	0.16	-0.41	62,81,95,101	0

6.5 Other polymers (i)

There are no such residues in this entry.