Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:18 PM GMT

PDB ID	:	1WYU
Title	:	Crystal structure of glycine decarboxylase (P-protein) of the glycine cleavage system, in holo form
Authors	:	Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-02-17
Resolution	:	2.10 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:

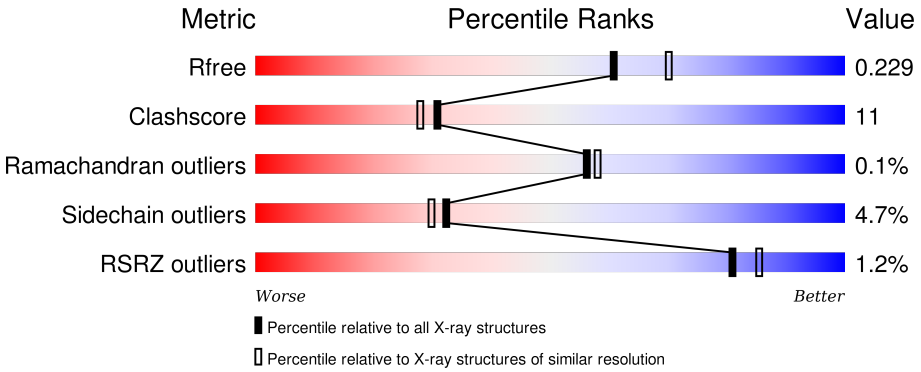
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	438	81% 16%
1	C	438	79% 19%
1	E	438	82% 16%
1	G	438	80% 18%
2	B	474	74% 23%

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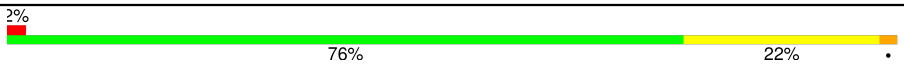
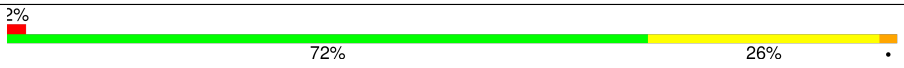
Mol	Chain	Length	Quality of chain
2	D	474	
2	F	474	
2	H	474	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30337 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.

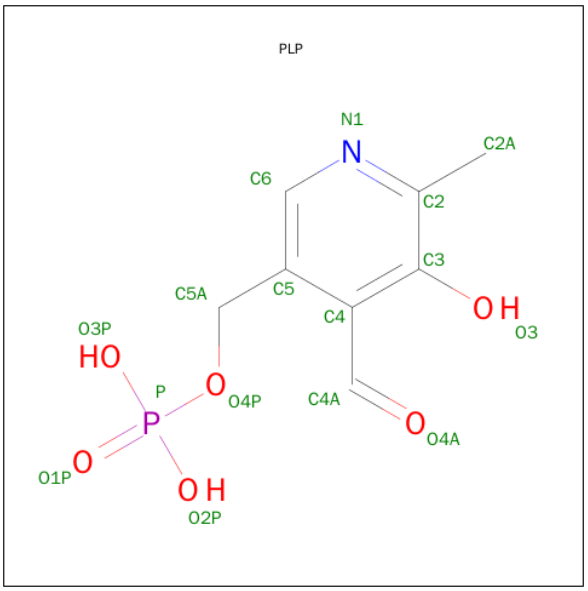
- Molecule 1 is a protein called glycine dehydrogenase (decarboxylating) subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	C	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	E	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	G	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			

- Molecule 2 is a protein called glycine dehydrogenase subunit 2 (P-protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	D	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	F	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			
2	H	473	Total	C	N	O	S	0	0	0
			3713	2380	655	666	12			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 15 8 1 5 1	0	0
3	D	1	Total C N O P 15 8 1 5 1	0	0
3	F	1	Total C N O P 15 8 1 5 1	0	0
3	H	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 4 is water.

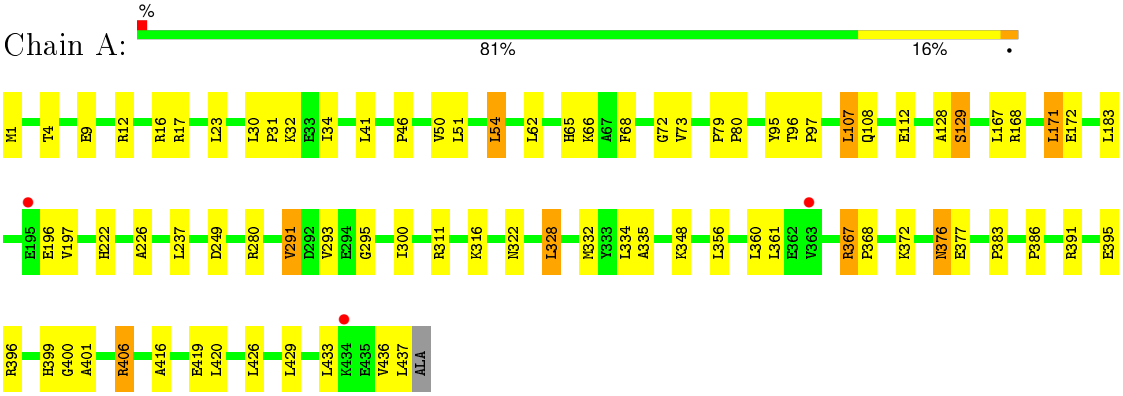
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	281	Total O 281 281	0	0
4	B	286	Total O 286 286	0	0
4	C	277	Total O 277 277	0	0
4	D	233	Total O 233 233	0	0
4	E	283	Total O 283 283	0	0
4	F	272	Total O 272 272	0	0
4	G	286	Total O 286 286	0	0
4	H	227	Total O 227 227	0	0

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.

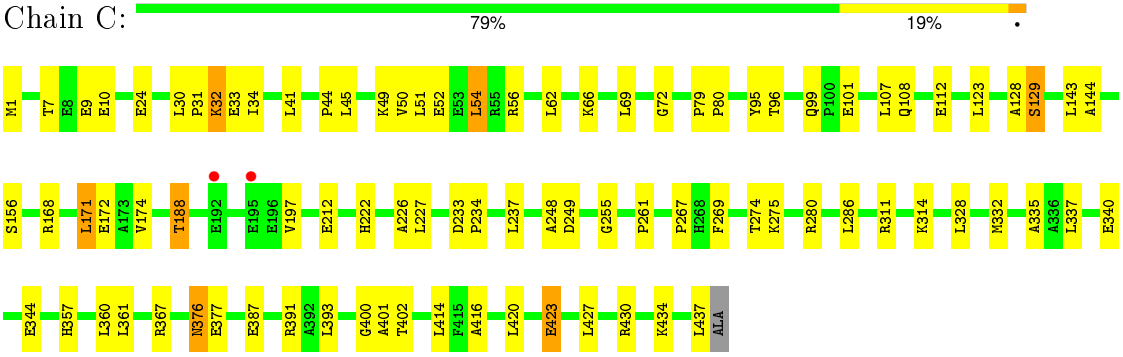
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

Chain A:



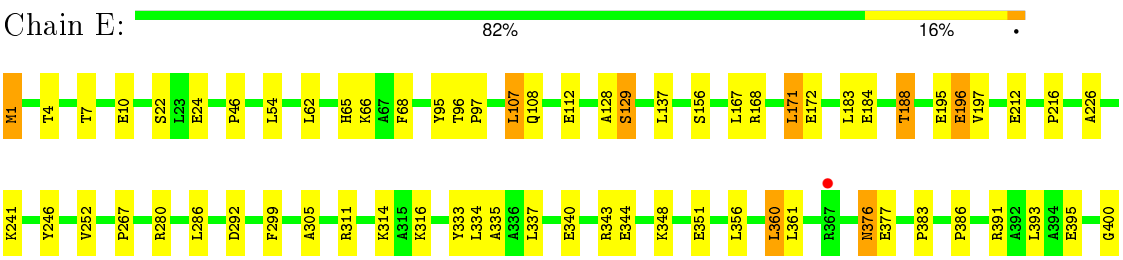
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

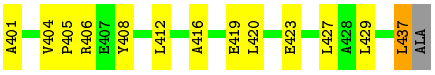
Chain C:



- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

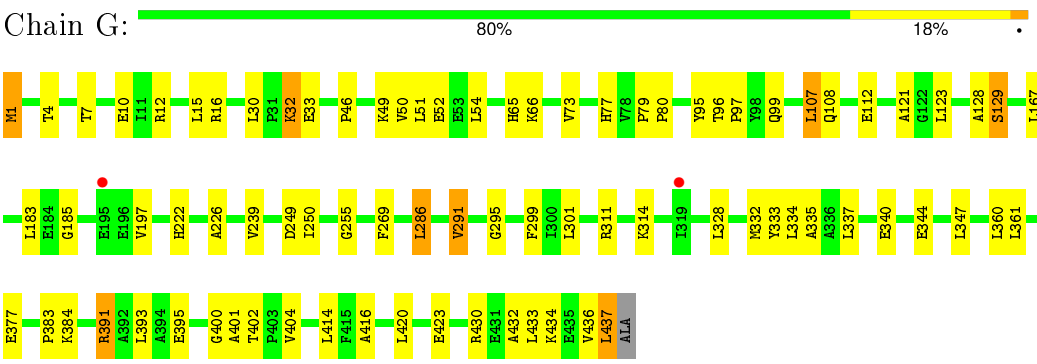
Chain E:





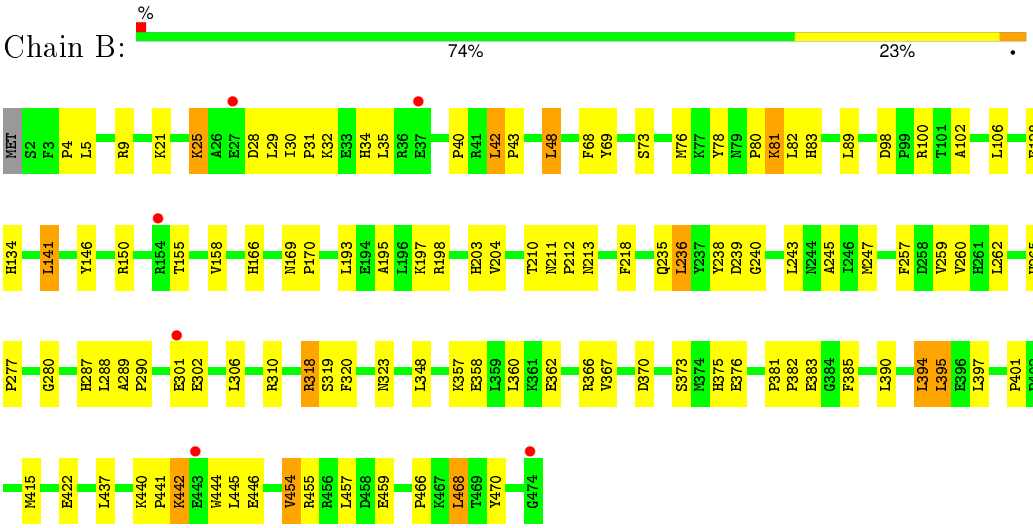
• Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

Chain G:



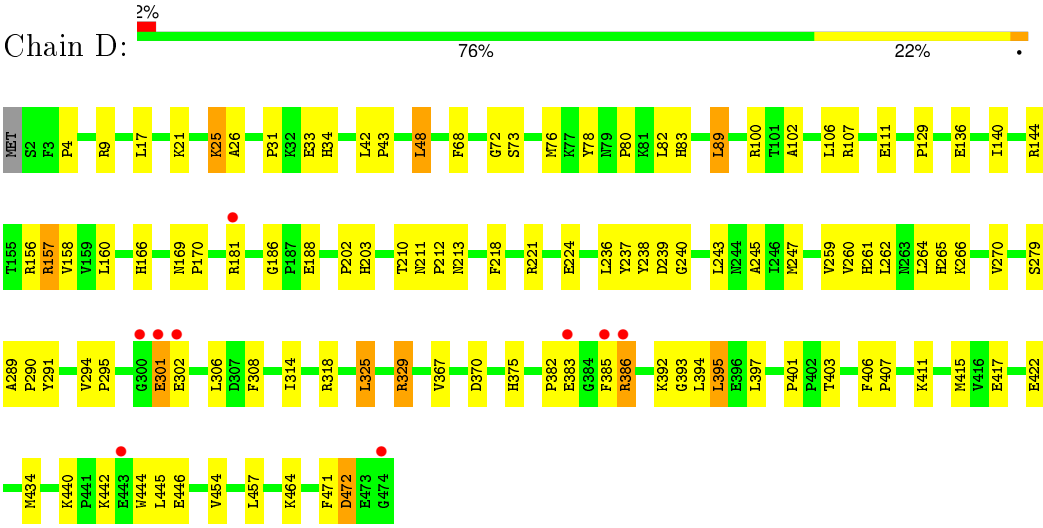
• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain B:



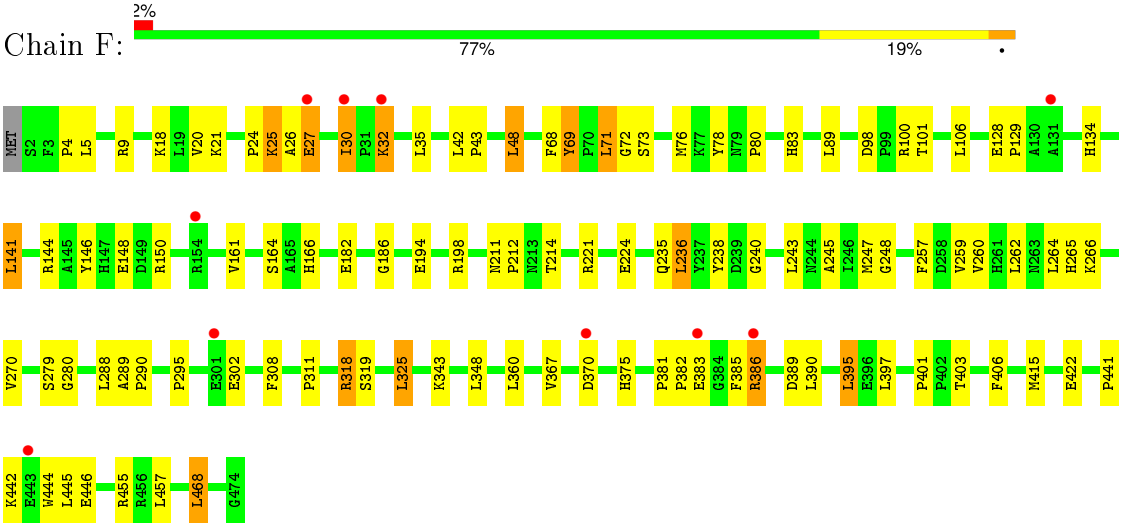
• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain D:



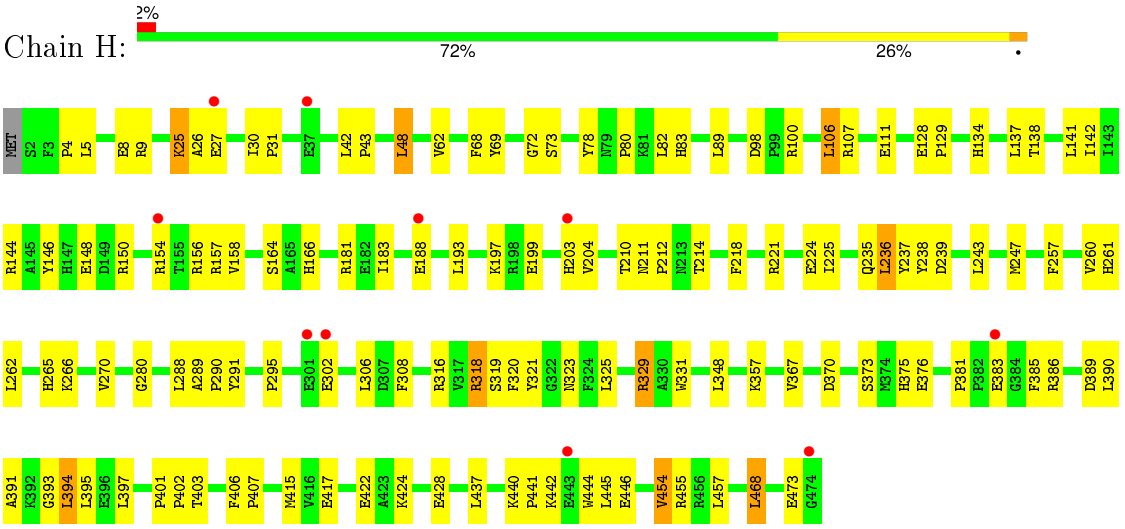
• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain F:



• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.87Å 166.67Å 189.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.10 49.57 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.57-2.10) 97.9 (49.57-2.09)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.229 0.189 , 0.229	Depositor DCC
R_{free} test set	12275 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 245447 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30337	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.32	0/3395	0.59	0/4617
1	C	0.31	0/3395	0.58	0/4617
1	E	0.32	0/3395	0.58	0/4617
1	G	0.32	0/3395	0.58	0/4617
2	B	0.35	1/3808 (0.0%)	0.61	0/5162
2	D	0.33	1/3808 (0.0%)	0.59	0/5162
2	F	0.34	1/3808 (0.0%)	0.60	0/5162
2	H	0.33	1/3808 (0.0%)	0.59	0/5162
All	All	0.33	4/28812 (0.0%)	0.59	0/39116

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	266	LYS	CE-NZ	-8.18	1.28	1.49
2	B	266	LYS	CE-NZ	-8.03	1.28	1.49
2	H	266	LYS	CE-NZ	-7.84	1.29	1.49
2	F	266	LYS	CE-NZ	-7.77	1.29	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3363	67	0
1	C	3320	0	3363	65	0
1	E	3320	0	3363	65	0
1	G	3320	0	3363	74	0
2	B	3713	0	3742	102	0
2	D	3713	0	3742	103	0
2	F	3713	0	3742	85	0
2	H	3713	0	3742	109	0
3	B	15	0	7	1	0
3	D	15	0	6	1	0
3	F	15	0	6	1	0
3	H	15	0	7	1	0
4	A	281	0	0	4	0
4	B	286	0	0	2	0
4	C	277	0	0	6	0
4	D	233	0	0	3	0
4	E	283	0	0	6	0
4	F	272	0	0	6	0
4	G	286	0	0	3	0
4	H	227	0	0	4	0
All	All	30337	0	28446	615	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 11.

All (615) 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:D:442:LYS:H	2:D:442:LYS:HD2	1.17	1.09
1:C:32:LYS:HD2	1:C:32:LYS:H	1.19	1.02
2:F:30:ILE:HD11	2:F:35:LEU:HD21	1.41	0.99
2:B:235:GLN:HE22	2:B:287:HIS:HE1	1.10	0.92
1:G:32:LYS:H	1:G:32:LYS:HD3	1.39	0.85
1:C:335:ALA:HA	2:D:43:PRO:HG2	1.58	0.85
1:E:128:ALA:O	1:E:129:SER:HB2	1.76	0.82
2:B:442:LYS:HD2	2:B:442:LYS:H	1.46	0.81
2:B:25:LYS:HA	2:B:25:LYS:HE2	1.61	0.81
2:D:25:LYS:HE3	2:D:26:ALA:H	1.43	0.81
1:E:335:ALA:HA	2:F:43:PRO:HG2	1.64	0.80
1:G:335:ALA:HA	2:H:43:PRO:HG2	1.63	0.80
1:A:436:VAL:HG23	1:A:437:LEU:HD13	1.64	0.79
2:D:442:LYS:N	2:D:442:LYS:HD2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:265:HIS:HA	2:F:270:VAL:HB	1.62	0.78
2:H:238:TYR:HB3	2:H:260:VAL:HG22	1.66	0.77
2:H:164:SER:O	2:H:214:THR:HG21	1.84	0.77
2:H:25:LYS:HE3	2:H:26:ALA:H	1.49	0.76
2:D:265:HIS:HA	2:D:270:VAL:HB	1.65	0.76
2:D:383:GLU:CD	2:D:383:GLU:H	1.87	0.76
1:C:66:LYS:HG2	1:C:420:LEU:HD13	1.68	0.76
2:B:80:PRO:HG2	2:B:83:HIS:CE1	2.21	0.76
1:E:156:SER:OG	1:E:188:THR:HG21	1.87	0.75
2:H:25:LYS:HG3	2:H:27:GLU:HG2	1.70	0.74
2:F:80:PRO:HG2	2:F:83:HIS:CE1	2.24	0.73
1:A:32:LYS:HD3	1:A:32:LYS:H	1.53	0.73
2:H:164:SER:HB2	2:H:214:THR:CG2	2.19	0.72
1:A:32:LYS:H	1:A:32:LYS:CD	2.02	0.72
2:B:383:GLU:H	2:B:383:GLU:CD	1.92	0.72
1:G:97:PRO:HG2	1:G:301:LEU:HD21	1.72	0.72
1:C:32:LYS:HD2	1:C:32:LYS:N	2.00	0.72
2:B:310:ARG:HD2	4:B:499:HOH:O	1.88	0.71
2:B:235:GLN:HE22	2:B:287:HIS:CE1	2.02	0.71
2:F:68:PHE:CE1	2:F:422:GLU:HG3	2.26	0.71
1:E:1:MET:HG2	1:E:46:PRO:HA	1.71	0.71
1:E:391:ARG:HG3	1:E:391:ARG:HH11	1.56	0.71
2:F:383:GLU:CD	2:F:383:GLU:H	1.93	0.71
1:C:234:PRO:HA	1:C:237:LEU:HD23	1.73	0.70
2:D:442:LYS:CD	2:D:442:LYS:H	1.94	0.70
2:F:386:ARG:N	2:F:386:ARG:HD3	2.07	0.70
2:H:238:TYR:HD2	2:H:260:VAL:HG13	1.57	0.69
2:F:25:LYS:HA	2:F:25:LYS:HE2	1.72	0.69
2:H:80:PRO:HG2	2:H:83:HIS:CE1	2.28	0.69
2:H:440:LYS:HB2	2:H:445:LEU:HD21	1.75	0.69
2:H:25:LYS:HE3	2:H:26:ALA:N	2.07	0.69
2:F:129:PRO:HG2	2:F:280:GLY:O	1.93	0.68
2:F:72:GLY:HA3	2:F:415:MET:HG2	1.75	0.68
1:E:391:ARG:NH1	2:F:100:ARG:HD2	2.09	0.68
2:B:358:GLU:O	2:B:362:GLU:HG3	1.94	0.68
1:C:99:GLN:HG3	2:D:395:LEU:HD21	1.75	0.67
2:D:395:LEU:HD13	2:D:401:PRO:HD3	1.77	0.67
1:E:340:GLU:O	1:E:344:GLU:HG3	1.94	0.67
1:C:377:GLU:HG2	1:C:416:ALA:HB2	1.76	0.67
2:B:68:PHE:CE1	2:B:422:GLU:HG3	2.29	0.67
2:D:157:ARG:HE	2:D:157:ARG:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:LYS:H	1:G:32:LYS:CD	2.07	0.66
2:H:158:VAL:HG22	2:H:203:HIS:O	1.96	0.66
2:D:367:VAL:CG1	2:D:370:ASP:HB3	2.26	0.66
1:G:377:GLU:HG2	1:G:416:ALA:HB2	1.78	0.66
1:A:66:LYS:HG2	1:A:420:LEU:HD13	1.78	0.66
2:H:318:ARG:HD3	2:H:319:SER:O	1.95	0.66
2:H:221:ARG:HA	2:H:221:ARG:HE	1.62	0.66
2:B:367:VAL:CG1	2:B:370:ASP:HB3	2.26	0.65
1:A:335:ALA:HA	2:B:43:PRO:HG2	1.76	0.65
1:G:50:VAL:O	1:G:54:LEU:HD23	1.96	0.65
1:G:99:GLN:HG3	2:H:395:LEU:HD21	1.77	0.65
2:B:265:HIS:HA	2:B:270:VAL:HB	1.77	0.65
2:D:294:VAL:CG2	2:D:308:PHE:HA	2.28	0.64
2:B:158:VAL:HG12	2:B:203:HIS:O	1.98	0.64
2:D:83:HIS:HB3	2:D:329:ARG:HD2	1.80	0.64
1:G:107:LEU:HD11	1:G:301:LEU:CD2	2.28	0.64
1:G:77:HIS:HB2	1:G:420:LEU:HD21	1.79	0.64
1:E:188:THR:HG23	1:E:212:GLU:CD	2.18	0.64
2:D:221:ARG:NH2	2:D:224:GLU:HG3	2.13	0.64
2:D:442:LYS:O	2:D:446:GLU:HG3	1.98	0.63
2:F:26:ALA:O	2:F:30:ILE:HD13	1.99	0.63
2:B:243:LEU:HD13	2:B:247:MET:HB3	1.81	0.63
2:D:464:LYS:HA	2:D:464:LYS:HE2	1.79	0.63
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.63	0.63
2:D:144:ARG:O	2:D:148:GLU:HG3	1.98	0.63
2:B:195:ALA:O	2:B:198:ARG:HG2	1.98	0.63
1:E:128:ALA:O	1:E:129:SER:CB	2.47	0.63
1:G:1:MET:HG2	1:G:46:PRO:HA	1.81	0.62
2:H:4:PRO:HG2	2:H:9:ARG:NH2	2.14	0.62
2:B:198:ARG:HB3	2:B:198:ARG:NH1	2.13	0.62
2:H:129:PRO:HG2	2:H:280:GLY:O	2.00	0.62
2:D:386:ARG:NE	2:D:386:ARG:H	1.98	0.62
1:A:377:GLU:HG2	1:A:416:ALA:HB2	1.81	0.62
2:F:144:ARG:O	2:F:148:GLU:HG3	2.00	0.62
2:H:243:LEU:HD13	2:H:243:LEU:O	1.99	0.62
1:C:430:ARG:O	1:C:434:LYS:HG3	2.00	0.62
2:H:383:GLU:CD	2:H:383:GLU:H	2.03	0.62
2:D:80:PRO:HG2	2:D:83:HIS:CE1	2.35	0.62
2:D:301:GLU:HG2	2:D:302:GLU:OE2	2.00	0.62
2:H:166:HIS:HB2	3:H:475:PLP:H2A3	1.82	0.62
2:D:25:LYS:HE3	2:D:26:ALA:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:ILE:HD11	2:F:35:LEU:CD2	2.26	0.61
2:D:129:PRO:HG2	2:D:280:GLY:O	2.00	0.61
2:D:72:GLY:HA2	2:D:417:GLU:HB2	1.82	0.61
2:F:21:LYS:HB3	2:F:21:LYS:NZ	2.15	0.61
1:E:377:GLU:HG2	1:E:416:ALA:HB2	1.80	0.61
2:H:5:LEU:HB2	2:H:8:GLU:HG3	1.83	0.61
1:G:107:LEU:HD11	1:G:301:LEU:HD22	1.82	0.61
1:E:68:PHE:CD2	1:E:429:LEU:HD22	2.36	0.61
2:H:265:HIS:HA	2:H:270:VAL:HB	1.82	0.60
1:G:311:ARG:HG3	1:G:314:LYS:HB2	1.82	0.60
2:H:393:GLY:O	2:H:397:LEU:HD13	2.01	0.60
1:G:433:LEU:O	1:G:436:VAL:HG22	2.00	0.60
1:E:383:PRO:HG2	1:E:437:LEU:HG	1.83	0.60
2:B:48:LEU:HG	2:D:78:TYR:HB2	1.84	0.60
1:G:12:ARG:HG3	1:G:16:ARG:HH12	1.67	0.60
2:B:32:LYS:HD2	2:B:35:LEU:HD12	1.84	0.60
2:D:411:LYS:NZ	2:D:411:LYS:HB3	2.17	0.60
1:A:32:LYS:N	1:A:32:LYS:HD3	2.15	0.60
2:B:129:PRO:HG2	2:B:280:GLY:O	2.02	0.60
1:E:66:LYS:HG2	1:E:420:LEU:HD13	1.83	0.59
2:H:395:LEU:CD1	2:H:401:PRO:HD3	2.32	0.59
1:A:1:MET:HG3	1:A:46:PRO:HA	1.84	0.59
1:G:391:ARG:HD3	4:G:591:HOH:O	2.02	0.59
2:D:4:PRO:HG2	2:D:9:ARG:CZ	2.33	0.59
2:H:262:LEU:O	2:H:280:GLY:HA2	2.02	0.59
2:D:33:GLU:CD	2:D:33:GLU:H	2.05	0.59
2:H:83:HIS:HB3	2:H:329:ARG:HD2	1.85	0.59
2:D:243:LEU:HD13	2:D:243:LEU:O	2.03	0.59
2:F:221:ARG:NH2	2:F:224:GLU:HG3	2.18	0.59
2:B:78:TYR:HB2	2:D:48:LEU:HG	1.84	0.59
2:B:106:LEU:HD11	2:B:306:LEU:HD21	1.85	0.59
1:C:391:ARG:NH1	2:D:100:ARG:HD2	2.18	0.58
1:G:32:LYS:HG2	1:G:33:GLU:OE2	2.03	0.58
2:F:78:TYR:HB2	2:H:48:LEU:HG	1.85	0.58
1:E:168:ARG:O	1:E:172:GLU:HG3	2.03	0.58
2:B:158:VAL:HG13	2:B:204:VAL:HA	1.85	0.58
1:A:222:HIS:HE1	1:A:249:ASP:OD2	1.85	0.58
1:G:128:ALA:O	1:G:129:SER:CB	2.52	0.58
1:C:423:GLU:O	1:C:427:LEU:HD23	2.04	0.58
2:H:156:ARG:O	2:H:157:ARG:HD2	2.03	0.58
1:E:351:GLU:OE1	2:F:24:PRO:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ASP:OD2	2:H:100:ARG:HB2	2.04	0.58
2:F:403:THR:HB	2:F:415:MET:HB3	1.85	0.58
2:B:158:VAL:CG1	2:B:204:VAL:HA	2.34	0.58
1:E:311:ARG:HG3	1:E:314:LYS:HB2	1.85	0.58
1:G:30:LEU:HD22	2:H:218:PHE:CG	2.39	0.58
2:B:395:LEU:HD13	2:B:401:PRO:HD3	1.85	0.58
1:G:391:ARG:HH11	1:G:391:ARG:HG3	1.69	0.57
1:C:340:GLU:O	1:C:344:GLU:HG3	2.03	0.57
2:D:454:VAL:HG11	2:D:457:LEU:HD21	1.85	0.57
1:C:233:ASP:O	1:C:237:LEU:HD22	2.04	0.57
1:C:128:ALA:O	1:C:129:SER:CB	2.52	0.57
2:H:144:ARG:O	2:H:148:GLU:HG3	2.04	0.57
1:C:95:TYR:HB2	2:D:76:MET:CE	2.34	0.57
2:B:4:PRO:HG2	2:B:9:ARG:NH2	2.20	0.57
2:D:245:ALA:HB2	2:D:375:HIS:HB3	1.86	0.57
2:B:442:LYS:HD2	2:B:442:LYS:N	2.17	0.57
2:B:442:LYS:H	2:B:442:LYS:CD	2.10	0.57
2:H:68:PHE:CE1	2:H:422:GLU:HG3	2.39	0.57
1:A:108:GLN:O	1:A:112:GLU:HG3	2.04	0.57
1:G:222:HIS:HE1	1:G:249:ASP:OD2	1.87	0.57
2:B:243:LEU:CD1	2:B:247:MET:HB3	2.34	0.57
2:D:243:LEU:CD1	2:D:247:MET:HG2	2.35	0.57
1:C:72:GLY:HA3	4:C:531:HOH:O	2.04	0.57
1:G:436:VAL:HG23	1:G:437:LEU:HD13	1.86	0.56
2:D:367:VAL:HG12	2:D:370:ASP:HB3	1.87	0.56
2:F:4:PRO:HG2	2:F:9:ARG:CZ	2.35	0.56
1:A:62:LEU:HD22	1:A:399:HIS:NE2	2.20	0.56
2:F:442:LYS:O	2:F:446:GLU:HG3	2.05	0.56
1:G:33:GLU:H	1:G:33:GLU:CD	2.07	0.56
2:H:4:PRO:HG2	2:H:9:ARG:CZ	2.35	0.56
2:F:236:LEU:HD22	2:F:257:PHE:CE1	2.40	0.56
2:F:386:ARG:H	2:F:386:ARG:HD3	1.70	0.56
2:H:403:THR:HB	2:H:415:MET:HB3	1.87	0.56
2:B:235:GLN:NE2	2:B:287:HIS:HE1	1.92	0.56
2:H:211:ASN:HA	2:H:212:PRO:C	2.25	0.56
2:F:318:ARG:HD3	2:F:319:SER:O	2.05	0.56
1:G:372:LYS:HB2	1:G:372:LYS:NZ	2.21	0.56
2:D:264:LEU:HD22	2:D:279:SER:HB3	1.88	0.56
1:G:128:ALA:O	1:G:129:SER:HB3	2.06	0.56
1:G:391:ARG:O	1:G:395:GLU:HG3	2.06	0.56
1:A:168:ARG:O	1:A:172:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:245:ALA:HB2	2:F:375:HIS:HB3	1.88	0.55
2:H:375:HIS:CE1	2:H:376:GLU:HG2	2.41	0.55
1:G:99:GLN:HG2	2:H:395:LEU:HD11	1.89	0.55
2:H:391:ALA:O	2:H:395:LEU:HD13	2.07	0.55
2:H:146:TYR:O	2:H:150:ARG:HG3	2.06	0.55
2:F:441:PRO:HG2	2:F:444:TRP:HB2	1.88	0.55
2:F:4:PRO:HG2	2:F:9:ARG:NH2	2.22	0.55
2:F:30:ILE:HD13	2:F:30:ILE:H	1.72	0.55
1:G:384:LYS:HD2	1:G:437:LEU:HD12	1.89	0.55
2:H:394:LEU:HD13	2:H:437:LEU:HD11	1.87	0.55
1:C:50:VAL:O	1:C:54:LEU:HD22	2.07	0.55
2:H:188:GLU:HB2	4:H:660:HOH:O	2.06	0.55
2:B:68:PHE:HE1	2:B:422:GLU:HG3	1.71	0.55
2:B:357:LYS:HE2	2:B:373:SER:OG	2.07	0.55
1:G:391:ARG:HG3	1:G:391:ARG:NH1	2.21	0.55
2:F:166:HIS:HB2	3:F:475:PLP:H2A3	1.88	0.54
2:H:442:LYS:O	2:H:446:GLU:HG3	2.07	0.54
2:H:441:PRO:HG2	2:H:444:TRP:HB2	1.88	0.54
2:H:289:ALA:N	2:H:290:PRO:HD2	2.22	0.54
2:F:68:PHE:HE1	2:F:422:GLU:HG3	1.71	0.54
2:F:243:LEU:CD1	2:F:247:MET:HB3	2.38	0.54
2:D:102:ALA:O	2:D:106:LEU:HD23	2.07	0.54
2:B:25:LYS:HA	2:B:25:LYS:CE	2.36	0.54
2:B:198:ARG:HH11	2:B:198:ARG:CB	2.21	0.54
1:A:1:MET:H1	1:A:1:MET:CE	2.21	0.54
1:A:128:ALA:O	1:A:129:SER:CB	2.55	0.54
1:E:167:LEU:HG	1:E:171:LEU:HD22	1.88	0.54
2:D:158:VAL:HG11	2:D:181:ARG:HG3	1.89	0.54
1:E:348:LYS:HE3	2:F:20:VAL:HG13	1.90	0.54
1:A:128:ALA:O	1:A:129:SER:HB3	2.07	0.53
1:A:406:ARG:HH11	1:A:406:ARG:HG2	1.72	0.53
1:G:12:ARG:HG3	1:G:16:ARG:NH1	2.23	0.53
1:E:65:HIS:O	1:E:66:LYS:HB2	2.09	0.53
1:C:144:ALA:HA	1:C:227:LEU:HD12	1.90	0.53
1:A:367:ARG:HG3	1:A:368:PRO:HD2	1.91	0.53
1:C:128:ALA:O	1:C:129:SER:HB3	2.09	0.53
2:D:289:ALA:N	2:D:290:PRO:HD2	2.23	0.53
2:D:31:PRO:HG2	2:D:34:HIS:HD2	1.74	0.53
2:D:464:LYS:HE2	2:D:464:LYS:CA	2.38	0.53
1:G:432:ALA:O	1:G:436:VAL:HG13	2.09	0.53
2:H:164:SER:HB2	2:H:214:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:H1	1:C:1:MET:CE	2.21	0.52
2:B:4:PRO:HG2	2:B:9:ARG:CZ	2.40	0.52
2:F:318:ARG:CD	2:F:319:SER:O	2.57	0.52
2:D:160:LEU:HD23	2:D:181:ARG:HB2	1.90	0.52
2:B:375:HIS:CE1	2:B:376:GLU:HG2	2.44	0.52
2:F:146:TYR:O	2:F:150:ARG:HG3	2.09	0.52
2:D:294:VAL:HG23	2:D:308:PHE:HA	1.91	0.52
1:A:391:ARG:O	1:A:395:GLU:HG3	2.10	0.52
2:F:265:HIS:CA	2:F:270:VAL:HB	2.37	0.52
1:E:65:HIS:CE1	1:E:66:LYS:HG3	2.45	0.52
1:A:391:ARG:HH11	1:A:391:ARG:HG3	1.75	0.52
1:A:376:ASN:H	1:A:376:ASN:HD22	1.57	0.52
1:C:108:GLN:O	1:C:112:GLU:HG3	2.09	0.52
2:D:31:PRO:HB2	2:D:33:GLU:OE2	2.09	0.52
2:F:367:VAL:CG1	2:F:370:ASP:HB3	2.40	0.52
2:D:72:GLY:HA3	2:D:415:MET:HG2	1.92	0.52
2:B:30:ILE:HB	2:B:35:LEU:HD21	1.92	0.52
1:C:32:LYS:CD	1:C:32:LYS:H	1.94	0.52
1:E:391:ARG:O	1:E:395:GLU:HG3	2.10	0.52
2:H:62:VAL:HG23	2:H:69:TYR:OH	2.10	0.52
1:C:7:THR:OG1	1:C:10:GLU:HG3	2.10	0.52
1:G:340:GLU:O	1:G:344:GLU:HG3	2.10	0.52
2:H:367:VAL:CG1	2:H:370:ASP:HB3	2.40	0.52
2:D:106:LEU:HD11	2:D:306:LEU:HD21	1.92	0.51
1:A:167:LEU:HG	1:A:171:LEU:HD22	1.91	0.51
1:A:17:ARG:NH2	2:B:362:GLU:OE1	2.43	0.51
1:G:12:ARG:HD3	4:G:721:HOH:O	2.10	0.51
2:F:318:ARG:HD3	2:F:319:SER:N	2.25	0.51
2:F:238:TYR:CE2	2:F:240:GLY:HA2	2.45	0.51
2:H:236:LEU:HD22	2:H:257:PHE:CE1	2.45	0.51
1:A:291:VAL:HG22	1:A:295:GLY:C	2.31	0.51
1:E:280:ARG:HD3	1:E:280:ARG:O	2.10	0.51
2:B:394:LEU:HD13	2:B:437:LEU:CD1	2.41	0.51
1:C:222:HIS:HE1	1:C:249:ASP:OD2	1.93	0.51
2:D:238:TYR:HB3	2:D:260:VAL:HG12	1.92	0.51
2:H:237:TYR:OH	2:H:261:HIS:HB3	2.11	0.51
1:A:32:LYS:H	1:A:32:LYS:CE	2.24	0.51
1:E:4:THR:HG21	2:F:348:LEU:HD12	1.93	0.51
2:B:442:LYS:O	2:B:446:GLU:HG3	2.11	0.51
2:B:301:GLU:OE1	2:B:301:GLU:HA	2.10	0.51
2:H:243:LEU:CD1	2:H:247:MET:HG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LYS:HE3	4:B:526:HOH:O	2.09	0.51
2:B:318:ARG:HD3	2:B:319:SER:O	2.10	0.50
1:C:314:LYS:NZ	1:C:314:LYS:HB3	2.25	0.50
2:D:31:PRO:HG2	2:D:34:HIS:CD2	2.46	0.50
1:E:280:ARG:NH1	1:E:316:LYS:NZ	2.59	0.50
1:E:65:HIS:HD2	4:F:732:HOH:O	1.94	0.50
2:H:394:LEU:HD13	2:H:437:LEU:CD1	2.41	0.50
1:A:376:ASN:H	1:A:376:ASN:ND2	2.10	0.50
2:F:243:LEU:HD13	2:F:247:MET:HB3	1.93	0.50
1:C:311:ARG:HG3	1:C:314:LYS:HB2	1.93	0.50
2:B:394:LEU:HD13	2:B:437:LEU:HD11	1.93	0.50
2:H:72:GLY:HA2	2:H:417:GLU:HB3	1.92	0.50
1:A:300:ILE:HD13	2:B:459:GLU:HG2	1.93	0.50
2:D:386:ARG:HE	2:D:386:ARG:H	1.60	0.50
2:H:72:GLY:HA3	2:H:415:MET:HG2	1.92	0.50
1:C:188:THR:HG23	1:C:212:GLU:CD	2.32	0.50
2:H:406:PHE:HA	2:H:407:PRO:C	2.32	0.50
2:D:4:PRO:HG2	2:D:9:ARG:NH2	2.26	0.49
1:C:30:LEU:HD22	2:D:218:PHE:CG	2.47	0.49
2:B:289:ALA:N	2:B:290:PRO:HD2	2.27	0.49
1:E:241:LYS:HD3	1:E:246:TYR:CZ	2.46	0.49
1:A:433:LEU:HA	1:A:436:VAL:HG22	1.93	0.49
1:C:212:GLU:HG3	4:C:696:HOH:O	2.12	0.49
2:H:381:PRO:HB3	2:H:390:LEU:CD1	2.43	0.49
2:F:48:LEU:HG	2:H:78:TYR:HB2	1.94	0.49
2:H:395:LEU:HD12	2:H:401:PRO:HD3	1.94	0.49
1:A:372:LYS:N	1:A:372:LYS:HD2	2.27	0.49
2:D:294:VAL:CG2	2:D:295:PRO:HA	2.42	0.49
2:H:260:VAL:HG12	2:H:261:HIS:N	2.26	0.49
2:D:301:GLU:N	2:D:301:GLU:OE1	2.45	0.49
2:B:31:PRO:HG2	2:B:34:HIS:HD2	1.77	0.49
2:D:188:GLU:HB2	4:D:616:HOH:O	2.13	0.49
1:A:376:ASN:N	1:A:376:ASN:HD22	2.11	0.48
2:B:146:TYR:O	2:B:150:ARG:HG3	2.12	0.48
1:A:356:LEU:HB2	1:A:426:LEU:HD22	1.95	0.48
1:A:300:ILE:CD1	2:B:459:GLU:HG2	2.42	0.48
1:G:108:GLN:O	1:G:112:GLU:HG3	2.13	0.48
2:H:107:ARG:O	2:H:111:GLU:HG3	2.12	0.48
2:F:161:VAL:O	2:F:182:GLU:HA	2.13	0.48
1:E:196:GLU:CD	1:E:196:GLU:H	2.17	0.48
2:H:158:VAL:CG2	2:H:204:VAL:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:ARG:NH1	1:E:391:ARG:HG3	2.27	0.48
1:E:108:GLN:O	1:E:112:GLU:HG3	2.14	0.48
1:E:22:SER:OG	1:E:24:GLU:HG2	2.14	0.48
2:D:454:VAL:CG1	2:D:457:LEU:HD21	2.43	0.48
2:H:210:THR:HG22	2:H:239:ASP:HB3	1.95	0.48
1:E:7:THR:OG1	1:E:10:GLU:HG3	2.14	0.48
1:G:430:ARG:O	1:G:434:LYS:HG3	2.14	0.48
2:D:136:GLU:O	2:D:140:ILE:HG12	2.14	0.48
2:F:32:LYS:HE3	2:F:35:LEU:HB2	1.96	0.48
2:B:134:HIS:HE1	2:B:318:ARG:HB3	1.79	0.48
1:G:49:LYS:HE3	1:G:52:GLU:OE1	2.14	0.48
2:F:128:GLU:N	2:F:129:PRO:HD2	2.29	0.47
2:B:238:TYR:HB3	2:B:260:VAL:HG12	1.95	0.47
2:F:381:PRO:HB3	2:F:390:LEU:CD1	2.44	0.47
2:B:166:HIS:HB2	3:B:475:PLP:H2A3	1.96	0.47
2:D:370:ASP:HA	4:D:594:HOH:O	2.13	0.47
2:B:367:VAL:HG12	2:B:370:ASP:HB3	1.96	0.47
1:C:45:LEU:HD22	1:C:49:LYS:HG2	1.97	0.47
1:G:197:VAL:O	1:G:226:ALA:HB2	2.14	0.47
2:B:245:ALA:HB2	2:B:375:HIS:HB3	1.94	0.47
1:G:291:VAL:HG22	1:G:295:GLY:C	2.34	0.47
2:D:264:LEU:HD22	2:D:279:SER:CB	2.43	0.47
2:D:393:GLY:O	2:D:397:LEU:HD13	2.14	0.47
2:F:455:ARG:HB3	4:F:579:HOH:O	2.14	0.47
2:B:454:VAL:HG11	2:B:457:LEU:HD21	1.97	0.47
2:F:238:TYR:HB3	2:F:260:VAL:HG12	1.97	0.47
1:E:216:PRO:HG2	4:E:592:HOH:O	2.14	0.47
1:C:168:ARG:O	1:C:172:GLU:HG3	2.14	0.47
1:C:69:LEU:HA	4:C:592:HOH:O	2.14	0.47
1:E:333:TYR:CE1	1:E:337:LEU:HD12	2.48	0.47
1:G:402:THR:HB	1:G:414:LEU:HB2	1.96	0.47
2:D:169:ASN:HB2	2:D:170:PRO:CD	2.45	0.47
2:D:291:TYR:O	2:D:314:ILE:HG23	2.15	0.47
2:B:98:ASP:OD2	2:B:100:ARG:HB2	2.14	0.47
1:A:386:PRO:HG2	4:A:671:HOH:O	2.15	0.47
1:A:73:VAL:HG23	2:B:320:PHE:CZ	2.50	0.47
1:G:239:VAL:HG21	1:G:347:LEU:HD21	1.96	0.47
1:E:137:LEU:HA	1:E:252:VAL:HG21	1.97	0.47
1:E:212:GLU:HG3	4:E:648:HOH:O	2.14	0.47
1:E:343:ARG:HH22	2:F:25:LYS:NZ	2.13	0.47
1:G:1:MET:N	1:G:1:MET:SD	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:454:VAL:HG11	2:H:457:LEU:HD21	1.96	0.47
1:G:65:HIS:O	1:G:66:LYS:HB2	2.15	0.47
2:H:158:VAL:HG23	2:H:204:VAL:HA	1.96	0.47
2:B:29:LEU:N	2:B:29:LEU:HD22	2.29	0.47
1:A:293:VAL:HG12	2:B:455:ARG:HB2	1.97	0.47
2:B:381:PRO:HB3	2:B:390:LEU:CD1	2.45	0.47
2:F:21:LYS:HB3	2:F:21:LYS:HZ2	1.81	0.47
2:F:318:ARG:NE	4:F:626:HOH:O	2.25	0.47
2:H:137:LEU:O	2:H:141:LEU:HD13	2.15	0.47
1:E:95:TYR:CG	1:E:96:THR:N	2.83	0.47
2:D:325:LEU:O	2:D:329:ARG:HG2	2.15	0.46
1:E:65:HIS:ND1	1:E:66:LYS:HG3	2.30	0.46
1:A:12:ARG:HH11	1:A:12:ARG:HG2	1.80	0.46
2:F:386:ARG:HG2	2:F:389:ASP:OD2	2.15	0.46
2:H:221:ARG:HA	2:H:221:ARG:NE	2.29	0.46
1:A:46:PRO:HD3	2:D:21:LYS:HG2	1.97	0.46
1:E:97:PRO:HG3	1:E:107:LEU:HD13	1.97	0.46
1:E:376:ASN:H	1:E:376:ASN:HD22	1.64	0.46
1:A:348:LYS:HG3	1:A:419:GLU:HA	1.98	0.46
2:B:403:THR:HB	2:B:415:MET:HB3	1.96	0.46
2:D:262:LEU:O	2:D:280:GLY:HA2	2.15	0.46
1:G:7:THR:OG1	1:G:10:GLU:HG3	2.15	0.46
1:E:299:PHE:CZ	2:F:5:LEU:HD21	2.50	0.46
2:H:80:PRO:CG	2:H:83:HIS:CE1	2.98	0.46
1:A:95:TYR:HB2	2:B:76:MET:CE	2.46	0.46
2:B:211:ASN:HA	2:B:212:PRO:C	2.35	0.46
2:D:265:HIS:CA	2:D:270:VAL:HB	2.40	0.46
1:E:188:THR:HG23	1:E:212:GLU:OE1	2.15	0.46
2:D:302:GLU:CD	2:D:302:GLU:H	2.18	0.46
1:E:400:GLY:O	1:E:401:ALA:HB3	2.15	0.46
1:E:280:ARG:NH1	1:E:316:LYS:HZ1	2.12	0.46
1:C:9:GLU:H	1:C:9:GLU:CD	2.18	0.46
1:E:195:GLU:HG2	4:E:704:HOH:O	2.16	0.46
2:H:142:ILE:HG23	2:H:291:TYR:HB2	1.98	0.46
2:H:193:LEU:O	2:H:197:LYS:HG3	2.16	0.46
2:B:40:PRO:HG2	2:B:42:LEU:HD22	1.98	0.46
1:E:391:ARG:CG	1:E:391:ARG:HH11	2.27	0.46
2:B:394:LEU:HD23	2:B:401:PRO:HA	1.97	0.46
1:C:156:SER:OG	1:C:188:THR:HG21	2.16	0.46
2:B:31:PRO:HG2	2:B:34:HIS:CD2	2.50	0.46
2:F:235:GLN:HE21	2:F:288:LEU:HD11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:ILE:HG23	2:H:31:PRO:HD2	1.97	0.46
2:F:262:LEU:O	2:F:280:GLY:HA2	2.16	0.46
2:D:294:VAL:HG23	2:D:295:PRO:HA	1.98	0.46
2:B:444:TRP:CE3	2:B:445:LEU:HD12	2.51	0.46
2:D:471:PHE:O	2:D:472:ASP:C	2.55	0.46
1:E:95:TYR:HB2	2:F:76:MET:CE	2.46	0.45
1:C:357:HIS:O	1:C:361:LEU:HD13	2.16	0.45
1:C:143:LEU:HD23	1:C:143:LEU:C	2.37	0.45
2:H:386:ARG:HG2	2:H:389:ASP:OD2	2.17	0.45
1:G:50:VAL:O	1:G:54:LEU:CD2	2.63	0.45
2:H:138:THR:O	2:H:142:ILE:HG13	2.16	0.45
1:C:101:GLU:CD	2:D:392:LYS:HZ2	2.19	0.45
1:C:51:LEU:HG	2:D:82:LEU:HD11	1.98	0.45
2:H:325:LEU:O	2:H:329:ARG:HG2	2.16	0.45
2:H:306:LEU:HD22	2:H:306:LEU:N	2.31	0.45
1:G:299:PHE:CZ	2:H:5:LEU:HD21	2.51	0.45
2:D:210:THR:CG2	2:D:239:ASP:HB3	2.47	0.45
1:A:376:ASN:ND2	4:A:526:HOH:O	2.50	0.45
1:A:280:ARG:NH2	1:A:311:ARG:HH22	2.13	0.45
1:A:322:ASN:O	2:B:277:PRO:HA	2.16	0.45
2:F:395:LEU:HD13	2:F:401:PRO:HD3	1.98	0.45
1:A:433:LEU:O	1:A:436:VAL:HG22	2.16	0.45
1:G:301:LEU:HD23	4:G:504:HOH:O	2.16	0.45
2:B:382:PRO:HG2	2:B:385:PHE:CD1	2.52	0.45
2:F:26:ALA:HB1	2:F:35:LEU:HD21	1.98	0.45
2:D:294:VAL:HG21	2:D:308:PHE:HA	1.98	0.45
2:B:262:LEU:O	2:B:280:GLY:HA2	2.16	0.45
2:F:382:PRO:HG2	2:F:385:PHE:CD1	2.52	0.45
1:E:305:ALA:HB3	4:E:678:HOH:O	2.16	0.45
1:A:4:THR:HG21	2:B:348:LEU:HD12	1.98	0.45
2:F:211:ASN:HA	2:F:212:PRO:C	2.37	0.45
1:G:95:TYR:CG	1:G:96:THR:N	2.85	0.45
1:G:121:ALA:HB1	1:G:123:LEU:HD23	1.98	0.45
1:A:51:LEU:HG	2:B:82:LEU:HD11	1.97	0.45
2:H:455:ARG:HB3	4:H:548:HOH:O	2.16	0.45
1:A:383:PRO:HG2	1:A:437:LEU:HG	1.99	0.45
1:G:12:ARG:NE	1:G:16:ARG:HH12	2.15	0.45
1:C:197:VAL:O	1:C:226:ALA:HB2	2.17	0.45
1:A:31:PRO:HG2	1:A:34:ILE:HG12	1.99	0.45
1:C:261:PRO:HG2	4:C:502:HOH:O	2.17	0.45
2:B:210:THR:HG22	2:B:239:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:LYS:HD3	2:F:27:GLU:HG3	1.99	0.44
2:B:236:LEU:HD22	2:B:257:PHE:CE1	2.52	0.44
2:D:25:LYS:HA	2:D:25:LYS:HE3	1.98	0.44
1:A:400:GLY:O	1:A:401:ALA:HB3	2.17	0.44
2:F:248:GLY:HA3	2:F:343:LYS:HG2	1.99	0.44
2:F:134:HIS:HE1	2:F:318:ARG:HB3	1.81	0.44
2:B:28:ASP:C	2:B:29:LEU:HD22	2.38	0.44
2:B:444:TRP:HE3	2:B:445:LEU:HD12	1.83	0.44
1:A:9:GLU:CD	1:A:9:GLU:H	2.20	0.44
1:A:66:LYS:HD2	4:C:657:HOH:O	2.17	0.44
2:B:318:ARG:NH2	2:B:323:ASN:OD1	2.50	0.44
1:A:95:TYR:CG	1:A:96:THR:N	2.85	0.44
1:E:197:VAL:O	1:E:226:ALA:HB2	2.17	0.44
1:E:348:LYS:HG3	1:E:419:GLU:HA	1.98	0.44
2:B:245:ALA:HB2	2:B:375:HIS:CG	2.53	0.44
1:C:95:TYR:CG	1:C:96:THR:N	2.86	0.44
2:B:210:THR:OG1	2:B:213:ASN:HA	2.17	0.44
1:C:255:GLY:HA3	1:C:269:PHE:CE1	2.52	0.44
1:A:396:ARG:HG3	1:A:396:ARG:HH11	1.83	0.44
2:H:402:PRO:HB2	2:H:415:MET:O	2.18	0.44
2:D:261:HIS:CD2	2:D:261:HIS:C	2.91	0.44
2:B:102:ALA:O	2:B:106:LEU:HD23	2.18	0.44
2:B:381:PRO:HB2	2:B:385:PHE:HB2	1.99	0.44
1:C:376:ASN:H	1:C:376:ASN:HD22	1.66	0.44
1:G:97:PRO:HB2	1:G:107:LEU:HD22	1.99	0.44
1:C:174:VAL:HG22	1:C:174:VAL:O	2.18	0.44
2:H:80:PRO:HG2	2:H:83:HIS:ND1	2.34	0.43
2:F:129:PRO:CG	2:F:280:GLY:O	2.62	0.43
1:C:400:GLY:O	1:C:401:ALA:HB3	2.18	0.43
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.31	0.43
2:B:198:ARG:NH1	2:B:198:ARG:CB	2.78	0.43
1:G:391:ARG:NH1	2:H:100:ARG:CZ	2.81	0.43
1:E:376:ASN:H	1:E:376:ASN:ND2	2.16	0.43
1:A:30:LEU:HD22	2:B:218:PHE:CG	2.53	0.43
1:C:248:ALA:O	1:C:275:LYS:HE3	2.19	0.43
2:B:466:PRO:HB2	2:B:468:LEU:CD1	2.48	0.43
2:H:394:LEU:HA	2:H:394:LEU:HD12	1.90	0.43
1:G:167:LEU:HG	1:G:171:LEU:HD22	2.00	0.43
1:C:79:PRO:HA	1:C:80:PRO:HD2	1.84	0.43
2:H:316:ARG:NH1	2:H:316:ARG:HG2	2.34	0.43
1:G:328:LEU:O	1:G:332:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:ILE:N	2:F:30:ILE:HD13	2.34	0.43
2:D:166:HIS:HB2	3:D:475:PLP:H2A3	2.01	0.43
2:F:30:ILE:HG12	2:F:35:LEU:HG	1.99	0.43
1:C:267:PRO:HD2	2:D:325:LEU:HB2	2.00	0.43
2:H:381:PRO:HB2	2:H:385:PHE:HB2	2.00	0.43
1:A:65:HIS:O	1:A:66:LYS:HB2	2.19	0.43
2:H:134:HIS:HE1	2:H:318:ARG:HB3	1.84	0.43
2:H:318:ARG:NH2	2:H:323:ASN:OD1	2.51	0.43
1:E:406:ARG:HD2	4:E:554:HOH:O	2.17	0.43
2:H:72:GLY:HA2	2:H:417:GLU:CB	2.49	0.43
2:H:210:THR:CG2	2:H:239:ASP:HB3	2.49	0.43
1:G:185:GLY:O	1:G:371:PRO:HG3	2.18	0.43
1:G:49:LYS:HD2	1:G:49:LYS:HA	1.83	0.43
1:G:255:GLY:HA3	1:G:269:PHE:CE1	2.54	0.43
2:H:154:ARG:HG3	2:H:154:ARG:HH11	1.84	0.43
1:G:383:PRO:HG2	1:G:437:LEU:HG	2.01	0.43
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.32	0.43
1:C:376:ASN:ND2	1:C:376:ASN:H	2.16	0.42
2:H:357:LYS:HD2	2:H:373:SER:OG	2.18	0.42
1:G:400:GLY:O	1:G:401:ALA:HB3	2.18	0.42
1:E:391:ARG:NH1	2:F:98:ASP:OD2	2.52	0.42
1:C:54:LEU:HB3	2:D:89:LEU:HD23	2.00	0.42
4:A:718:HOH:O	2:B:266:LYS:HE2	2.19	0.42
1:G:30:LEU:HD22	2:H:218:PHE:CD2	2.54	0.42
1:A:62:LEU:HD22	1:A:399:HIS:HE2	1.82	0.42
2:D:238:TYR:CE2	2:D:240:GLY:HA2	2.54	0.42
1:E:376:ASN:N	1:E:376:ASN:HD22	2.18	0.42
2:D:107:ARG:O	2:D:111:GLU:HG3	2.20	0.42
2:F:69:TYR:HD1	2:F:71:LEU:HD22	1.84	0.42
2:D:440:LYS:HG2	2:D:444:TRP:CE3	2.54	0.42
2:F:166:HIS:HA	2:F:406:PHE:CZ	2.54	0.42
1:E:299:PHE:HZ	2:F:5:LEU:HD21	1.85	0.42
1:G:4:THR:HG21	2:H:348:LEU:HD12	2.00	0.42
2:H:238:TYR:CB	2:H:260:VAL:HG22	2.44	0.42
2:F:68:PHE:CD1	2:F:422:GLU:HG3	2.54	0.42
2:D:72:GLY:HA2	2:D:417:GLU:CB	2.49	0.42
2:B:210:THR:CG2	2:B:239:ASP:HB3	2.50	0.42
1:C:328:LEU:O	1:C:332:MET:HG3	2.19	0.42
1:C:24:GLU:OE1	1:C:24:GLU:N	2.42	0.42
1:A:97:PRO:HG3	1:A:107:LEU:HD13	2.01	0.42
1:E:383:PRO:CG	1:E:437:LEU:HG	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE2	1:A:197:VAL:HG23	2.19	0.42
2:H:295:PRO:HB3	2:H:308:PHE:CE1	2.54	0.42
1:A:79:PRO:HA	1:A:80:PRO:HD2	1.85	0.42
2:B:406:PHE:HA	2:B:407:PRO:C	2.40	0.42
1:C:387:GLU:HG3	4:C:517:HOH:O	2.20	0.42
1:C:52:GLU:O	1:C:56:ARG:HG3	2.20	0.42
2:H:128:GLU:N	2:H:129:PRO:HD2	2.35	0.42
1:G:12:ARG:CD	1:G:16:ARG:HH12	2.33	0.42
2:B:238:TYR:CE2	2:B:240:GLY:HA2	2.55	0.42
2:B:441:PRO:HG2	2:B:444:TRP:HB2	2.02	0.42
2:H:106:LEU:HD11	2:H:306:LEU:HD21	2.01	0.42
2:D:68:PHE:CE1	2:D:422:GLU:HG3	2.55	0.42
2:H:181:ARG:HD2	2:H:199:GLU:OE1	2.20	0.42
2:D:382:PRO:HG2	2:D:385:PHE:CD1	2.54	0.42
2:D:403:THR:HB	2:D:415:MET:HB3	2.02	0.42
1:C:314:LYS:HZ2	1:C:314:LYS:HB3	1.84	0.42
2:B:169:ASN:HB2	2:B:170:PRO:CD	2.50	0.42
2:B:235:GLN:HE21	2:B:288:LEU:HD11	1.85	0.42
2:F:146:TYR:O	2:F:150:ARG:CG	2.68	0.42
1:G:171:LEU:HD23	1:G:178:LEU:HB2	2.02	0.41
1:C:402:THR:HB	1:C:414:LEU:HB2	2.02	0.41
1:G:311:ARG:HG3	1:G:314:LYS:CB	2.50	0.41
2:D:243:LEU:HD12	2:D:247:MET:HG2	2.00	0.41
2:D:259:VAL:HG23	2:D:284:VAL:HG12	2.02	0.41
2:B:238:TYR:HB2	2:B:257:PHE:CD1	2.55	0.41
2:D:211:ASN:HA	2:D:212:PRO:C	2.40	0.41
2:H:238:TYR:HB2	2:H:257:PHE:CD1	2.54	0.41
1:G:97:PRO:HG3	1:G:107:LEU:HD13	2.02	0.41
2:H:445:LEU:HD22	2:H:445:LEU:N	2.34	0.41
2:H:221:ARG:NH1	2:H:224:GLU:HG2	2.35	0.41
1:G:54:LEU:CD2	2:H:331:TRP:HZ3	2.33	0.41
1:G:404:VAL:CG2	1:G:414:LEU:HG	2.50	0.41
2:D:210:THR:OG1	2:D:213:ASN:HA	2.20	0.41
2:B:21:LYS:HE2	1:C:44:PRO:O	2.20	0.41
2:D:186:GLY:HA3	4:D:628:HOH:O	2.20	0.41
2:B:366:ARG:NH1	2:B:381:PRO:O	2.54	0.41
1:C:143:LEU:HD23	1:C:143:LEU:O	2.20	0.41
1:A:280:ARG:NH1	1:A:316:LYS:NZ	2.68	0.41
2:F:194:GLU:O	2:F:198:ARG:HD3	2.20	0.41
1:C:280:ARG:HH11	1:C:280:ARG:HG3	1.86	0.41
2:H:389:ASP:HB3	2:H:445:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:LEU:CD1	2:D:401:PRO:HD3	2.49	0.41
2:F:289:ALA:N	2:F:290:PRO:HD2	2.35	0.41
1:E:405:PRO:HG2	1:E:408:TYR:CD2	2.56	0.41
2:H:221:ARG:O	2:H:225:ILE:HG13	2.21	0.41
2:H:4:PRO:HB3	4:H:635:HOH:O	2.19	0.41
2:H:316:ARG:HH11	2:H:316:ARG:HG2	1.86	0.41
1:A:50:VAL:O	1:A:54:LEU:HD22	2.19	0.41
1:E:404:VAL:HB	1:E:412:LEU:HB2	2.02	0.41
2:F:311:PRO:HG2	4:F:573:HOH:O	2.19	0.41
1:E:356:LEU:HG	1:E:360:LEU:HD22	2.02	0.41
2:D:78:TYR:CZ	2:D:80:PRO:HA	2.56	0.41
2:F:264:LEU:HD22	2:F:279:SER:OG	2.21	0.41
2:F:468:LEU:HB3	4:F:497:HOH:O	2.19	0.41
1:C:337:LEU:HD13	2:D:17:LEU:HB2	2.02	0.41
1:G:286:LEU:CD2	2:H:468:LEU:HG	2.50	0.41
2:D:424:LYS:O	2:D:428:GLU:HG3	2.21	0.41
2:H:235:GLN:HE21	2:H:288:LEU:HD11	1.85	0.41
2:F:141:LEU:HD12	2:F:141:LEU:HA	1.85	0.41
1:A:328:LEU:O	1:A:332:MET:HG3	2.21	0.41
2:D:411:LYS:HZ3	2:D:411:LYS:HB3	1.85	0.41
1:E:267:PRO:HD2	2:F:325:LEU:HB2	2.01	0.41
2:D:406:PHE:HA	2:D:407:PRO:C	2.41	0.41
2:B:141:LEU:HD12	2:B:141:LEU:HA	1.94	0.41
1:A:72:GLY:HA3	4:A:647:HOH:O	2.20	0.41
2:H:260:VAL:CG1	2:H:261:HIS:N	2.83	0.41
2:B:80:PRO:HG2	2:B:83:HIS:ND1	2.36	0.41
2:B:155:THR:O	2:B:203:HIS:HA	2.20	0.41
2:H:370:ASP:HA	4:H:675:HOH:O	2.20	0.41
2:D:136:GLU:HA	2:D:237:TYR:OH	2.21	0.41
2:D:156:ARG:HD3	2:D:202:PRO:O	2.21	0.41
1:G:333:TYR:CE2	1:G:337:LEU:HD12	2.56	0.41
1:E:386:PRO:HG2	4:E:687:HOH:O	2.21	0.41
2:H:424:LYS:O	2:H:428:GLU:HG3	2.21	0.41
1:C:123:LEU:HD13	1:C:274:THR:HA	2.03	0.41
1:E:391:ARG:HA	2:F:98:ASP:OD2	2.21	0.41
2:D:245:ALA:HB2	2:D:375:HIS:CG	2.56	0.41
2:D:237:TYR:CD1	2:D:259:VAL:HG13	2.56	0.41
1:A:197:VAL:O	1:A:226:ALA:HB2	2.21	0.41
2:F:295:PRO:HB3	2:F:308:PHE:CE1	2.56	0.41
1:A:68:PHE:CD2	1:A:429:LEU:HD22	2.56	0.41
1:C:335:ALA:HA	2:D:43:PRO:CG	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ASP:C	1:G:250:ILE:HG13	2.40	0.40
2:D:102:ALA:O	2:D:106:LEU:CD2	2.69	0.40
1:G:73:VAL:HG23	2:H:320:PHE:CZ	2.56	0.40
2:B:193:LEU:O	2:B:197:LYS:HG3	2.21	0.40
2:B:357:LYS:NZ	2:B:370:ASP:HB2	2.35	0.40
2:B:25:LYS:HE2	2:B:25:LYS:CA	2.42	0.40
2:F:18:LYS:HB2	1:G:1:MET:HG3	2.03	0.40
1:E:377:GLU:HG2	1:E:416:ALA:CB	2.50	0.40
1:G:12:ARG:CG	1:G:16:ARG:HH12	2.31	0.40
2:B:128:GLU:N	2:B:129:PRO:HD2	2.36	0.40
1:A:280:ARG:HD3	1:A:280:ARG:O	2.21	0.40
2:F:186:GLY:HA3	4:F:638:HOH:O	2.21	0.40
1:E:62:LEU:HB3	2:F:101:THR:HB	2.04	0.40
2:F:164:SER:HB2	2:F:214:THR:OG1	2.22	0.40
2:B:5:LEU:HD13	2:B:470:TYR:HD1	1.86	0.40
2:D:203:HIS:H	2:D:203:HIS:CD2	2.37	0.40
1:G:51:LEU:HG	2:H:82:LEU:HD11	2.02	0.40
1:A:376:ASN:ND2	1:A:376:ASN:N	2.69	0.40
2:H:183:ILE:HG22	2:H:199:GLU:HG3	2.03	0.40
1:G:79:PRO:HA	1:G:80:PRO:HD2	1.88	0.40
1:A:436:VAL:HG23	1:A:437:LEU:CD1	2.44	0.40
1:G:372:LYS:HB2	1:G:372:LYS:HZ3	1.84	0.40
2:B:466:PRO:HB2	2:B:468:LEU:HD11	2.03	0.40
2:D:394:LEU:HD11	2:D:434:MET:SD	2.62	0.40
1:E:292:ASP:HA	2:F:457:LEU:HA	2.03	0.40
1:C:31:PRO:O	1:C:34:ILE:HG12	2.21	0.40
1:C:171:LEU:HD12	1:C:171:LEU:HA	1.89	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	435/438 (99%)	418 (96%)	16 (4%)	1 (0%)	52	53
1	C	435/438 (99%)	421 (97%)	13 (3%)	1 (0%)	52	53
1	E	435/438 (99%)	421 (97%)	13 (3%)	1 (0%)	52	53
1	G	435/438 (99%)	416 (96%)	18 (4%)	1 (0%)	52	53
2	B	471/474 (99%)	458 (97%)	13 (3%)	0	100	100
2	D	471/474 (99%)	455 (97%)	15 (3%)	1 (0%)	52	53
2	F	471/474 (99%)	453 (96%)	18 (4%)	0	100	100
2	H	471/474 (99%)	456 (97%)	15 (3%)	0	100	100
All	All	3624/3648 (99%)	3498 (96%)	121 (3%)	5 (0%)	56	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	C	129	SER
1	E	129	SER
1	G	129	SER
2	D	472	ASP

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	336/336 (100%)	320 (95%)	16 (5%)	31	29
1	C	336/336 (100%)	321 (96%)	15 (4%)	34	32
1	E	336/336 (100%)	319 (95%)	17 (5%)	29	26
1	G	336/336 (100%)	320 (95%)	16 (5%)	31	29
2	B	384/385 (100%)	364 (95%)	20 (5%)	29	25
2	D	384/385 (100%)	370 (96%)	14 (4%)	42	43
2	F	384/385 (100%)	361 (94%)	23 (6%)	24	20
2	H	384/385 (100%)	369 (96%)	15 (4%)	39	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2880/2884 (100%)	2744 (95%)	136 (5%)	32 30

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	23	LEU
1	A	41	LEU
1	A	54	LEU
1	A	107	LEU
1	A	171	LEU
1	A	183	LEU
1	A	237	LEU
1	A	291	VAL
1	A	328	LEU
1	A	334	LEU
1	A	360	LEU
1	A	361	LEU
1	A	367	ARG
1	A	376	ASN
1	A	406	ARG
2	B	25	LYS
2	B	42	LEU
2	B	48	LEU
2	B	69	TYR
2	B	73	SER
2	B	81	LYS
2	B	89	LEU
2	B	141	LEU
2	B	236	LEU
2	B	259	VAL
2	B	302	GLU
2	B	318	ARG
2	B	360	LEU
2	B	394	LEU
2	B	395	LEU
2	B	397	LEU
2	B	440	LYS
2	B	442	LYS
2	B	454	VAL
2	B	468	LEU
1	C	32	LYS

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Mol	Chain	Res	Type
1	C	33	GLU
1	C	41	LEU
1	C	54	LEU
1	C	62	LEU
1	C	107	LEU
1	C	171	LEU
1	C	188	THR
1	C	286	LEU
1	C	360	LEU
1	C	367	ARG
1	C	376	ASN
1	C	393	LEU
1	C	423	GLU
1	C	437	LEU
2	D	25	LYS
2	D	42	LEU
2	D	48	LEU
2	D	73	SER
2	D	89	LEU
2	D	157	ARG
2	D	236	LEU
2	D	301	GLU
2	D	318	ARG
2	D	325	LEU
2	D	329	ARG
2	D	386	ARG
2	D	395	LEU
2	D	445	LEU
1	E	1	MET
1	E	54	LEU
1	E	107	LEU
1	E	171	LEU
1	E	183	LEU
1	E	184	GLU
1	E	188	THR
1	E	196	GLU
1	E	286	LEU
1	E	334	LEU
1	E	360	LEU
1	E	361	LEU
1	E	376	ASN
1	E	393	LEU

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Mol	Chain	Res	Type
1	E	423	GLU
1	E	427	LEU
1	E	437	LEU
2	F	25	LYS
2	F	27	GLU
2	F	30	ILE
2	F	32	LYS
2	F	42	LEU
2	F	48	LEU
2	F	69	TYR
2	F	71	LEU
2	F	73	SER
2	F	89	LEU
2	F	106	LEU
2	F	141	LEU
2	F	236	LEU
2	F	259	VAL
2	F	302	GLU
2	F	318	ARG
2	F	325	LEU
2	F	360	LEU
2	F	386	ARG
2	F	395	LEU
2	F	397	LEU
2	F	445	LEU
2	F	468	LEU
1	G	1	MET
1	G	15	LEU
1	G	32	LYS
1	G	107	LEU
1	G	171	LEU
1	G	183	LEU
1	G	286	LEU
1	G	291	VAL
1	G	334	LEU
1	G	360	LEU
1	G	361	LEU
1	G	376	ASN
1	G	391	ARG
1	G	393	LEU
1	G	423	GLU
1	G	437	LEU

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Mol	Chain	Res	Type
2	H	25	LYS
2	H	42	LEU
2	H	48	LEU
2	H	73	SER
2	H	89	LEU
2	H	106	LEU
2	H	236	LEU
2	H	302	GLU
2	H	318	ARG
2	H	321	TYR
2	H	329	ARG
2	H	394	LEU
2	H	454	VAL
2	H	468	LEU
2	H	473	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	222	HIS
1	A	376	ASN
2	B	34	HIS
2	B	235	GLN
2	B	287	HIS
2	B	380	GLN
1	C	83	GLN
1	C	222	HIS
1	C	376	ASN
2	D	34	HIS
2	D	179	GLN
1	E	60	GLN
1	E	354	HIS
1	E	376	ASN
2	F	179	GLN
2	F	235	GLN
1	G	60	GLN
1	G	83	GLN
1	G	222	HIS
1	G	376	ASN
2	H	179	GLN
2	H	235	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLP	B	475	2	15,15,16	1.61	3 (20%)	21,22,23	2.12	3 (14%)
3	PLP	D	475	2	15,15,16	1.63	3 (20%)	21,22,23	2.14	3 (14%)
3	PLP	F	475	2	15,15,16	1.56	3 (20%)	21,22,23	2.09	3 (14%)
3	PLP	H	475	2	15,15,16	1.62	3 (20%)	21,22,23	2.05	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	B	475	2	-	0/6/6/8	0/1/1/1
3	PLP	D	475	2	-	0/6/6/8	0/1/1/1
3	PLP	F	475	2	-	0/6/6/8	0/1/1/1
3	PLP	H	475	2	-	0/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	475	PLP	C3-C2	-3.79	1.38	1.40
3	H	475	PLP	C3-C2	-3.29	1.38	1.40
3	B	475	PLP	C3-C2	-3.11	1.38	1.40
3	F	475	PLP	C3-C2	-2.77	1.38	1.40
3	F	475	PLP	C2-N1	2.20	1.38	1.34
3	D	475	PLP	C2-N1	2.27	1.38	1.34
3	H	475	PLP	C2-N1	2.33	1.39	1.34
3	B	475	PLP	C2-N1	2.36	1.39	1.34
3	D	475	PLP	C5-C4	2.83	1.43	1.40
3	F	475	PLP	C5-C4	3.00	1.44	1.40
3	H	475	PLP	C5-C4	3.01	1.44	1.40
3	B	475	PLP	C5-C4	3.03	1.44	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	475	PLP	C5-C6-N1	-2.28	119.90	123.86
3	H	475	PLP	C5-C6-N1	-2.26	119.93	123.86
3	D	475	PLP	C5-C6-N1	-2.26	119.94	123.86
3	F	475	PLP	C5-C6-N1	-2.13	120.17	123.86
3	B	475	PLP	C5A-C5-C4	2.69	125.21	121.65
3	H	475	PLP	C5A-C5-C4	2.76	125.31	121.65
3	F	475	PLP	C5A-C5-C4	2.79	125.35	121.65
3	D	475	PLP	C5A-C5-C4	2.79	125.35	121.65
3	H	475	PLP	O4P-C5A-C5	7.01	120.57	108.99
3	F	475	PLP	O4P-C5A-C5	7.30	121.07	108.99
3	B	475	PLP	O4P-C5A-C5	7.52	121.42	108.99
3	D	475	PLP	O4P-C5A-C5	7.58	121.52	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	475	PLP	1	0
3	D	475	PLP	1	0
3	F	475	PLP	1	0
3	H	475	PLP	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	437/438 (99%)	-0.22	3 (0%)	89	91	19, 26, 40, 48	0
1	C	437/438 (99%)	-0.29	2 (0%)	91	93	19, 27, 40, 47	0
1	E	437/438 (99%)	-0.28	1 (0%)	95	96	18, 25, 38, 49	0
1	G	437/438 (99%)	-0.30	2 (0%)	91	93	19, 26, 40, 48	0
2	B	473/474 (99%)	-0.21	7 (1%)	76	81	16, 24, 42, 57	0
2	D	473/474 (99%)	-0.17	10 (2%)	67	72	18, 29, 48, 63	0
2	F	473/474 (99%)	-0.19	10 (2%)	67	72	16, 25, 42, 52	0
2	H	473/474 (99%)	-0.16	10 (2%)	67	72	19, 30, 48, 61	0
All	All	3640/3648 (99%)	-0.23	45 (1%)	81	85	16, 27, 43, 63	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	301	GLU	4.8
2	B	301	GLU	3.8
2	D	302	GLU	3.7
2	F	386	ARG	3.7
2	H	154	ARG	3.5
2	H	302	GLU	3.3
2	B	474	GLY	3.3
2	D	301	GLU	3.1
2	D	474	GLY	3.1
2	D	386	ARG	3.0
2	H	383	GLU	2.9
2	F	370	ASP	2.9
2	D	154	ARG	2.9
1	C	195	GLU	2.8
2	B	443	GLU	2.8
2	B	37	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	27	GLU	2.8
2	D	383	GLU	2.7
2	B	154	ARG	2.6
2	H	188	GLU	2.5
1	G	195	GLU	2.4
2	F	443	GLU	2.4
2	F	30	ILE	2.3
2	D	443	GLU	2.3
2	B	131	ALA	2.3
2	H	27	GLU	2.2
2	H	443	GLU	2.2
2	F	301	GLU	2.2
2	D	385	PHE	2.2
2	D	181	ARG	2.2
2	H	203	HIS	2.2
2	H	37	GLU	2.2
2	D	300	GLY	2.1
1	E	367	ARG	2.1
2	B	27	GLU	2.1
2	F	383	GLU	2.1
1	G	319	ILE	2.1
1	A	195	GLU	2.1
1	C	192	GLU	2.1
2	F	131	ALA	2.1
2	H	474	GLY	2.1
1	A	363	VAL	2.1
1	A	434	LYS	2.0
2	F	154	ARG	2.0
2	F	32	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PLP	F	475	15/16	0.98	0.14	-0.02	18,26,31,31	0
3	PLP	H	475	15/16	0.97	0.12	-0.15	24,36,39,39	0
3	PLP	B	475	15/16	0.97	0.13	-0.31	21,31,34,35	0
3	PLP	D	475	15/16	0.96	0.11	-0.53	29,36,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.