



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:18 AM UTC

PDB ID : 3PBP / pdb_00003pbp
Title : Structure of the yeast heterotrimeric Nup82-Nup159-Nup116 nucleoporin complex
Authors : Debler, E.W.; Hoelz, A.
Deposited on : 2010-10-20
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

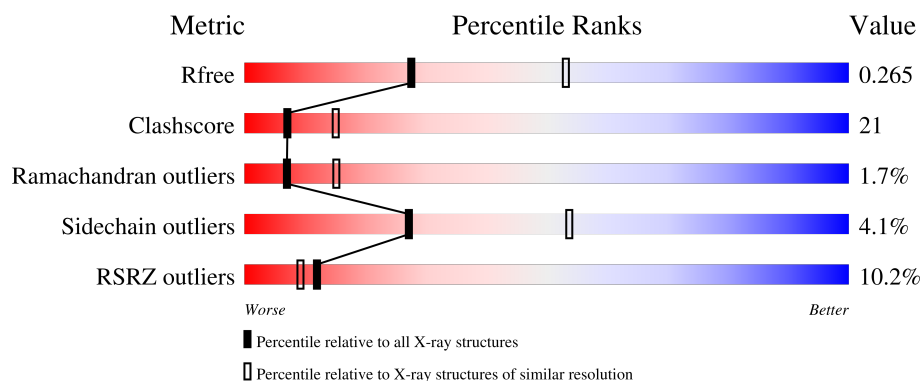
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	452	7% 58% 34% 5%
1	D	452	7% 57% 35% 5%
1	G	452	5% 58% 34% 5%
1	J	452	6% 58% 34% 5%
2	B	148	18% 57% 39% ••

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Mol	Chain	Length	Quality of chain
2	E	148	
2	H	148	
2	K	148	
3	C	36	
3	F	36	
3	I	36	
3	L	36	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PGE	D	6119	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19653 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 Nucleoporin NUP82.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	0	0
			3539	2273	569	686	4	7			
1	D	437	Total	C	N	O	S	Se	0	0	0
			3533	2270	568	684	4	7			
1	G	438	Total	C	N	O	S	Se	0	0	0
			3539	2273	569	686	4	7			
1	J	439	Total	C	N	O	S	Se	0	0	0
			3550	2279	573	687	4	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	CYS	engineered mutation	UNP P40368
D	396	SER	CYS	engineered mutation	UNP P40368
G	396	SER	CYS	engineered mutation	UNP P40368
J	396	SER	CYS	engineered mutation	UNP P40368

- Molecule 2 is a protein called Nucleoporin NUP116/NSP116.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	E	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	H	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	K	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			

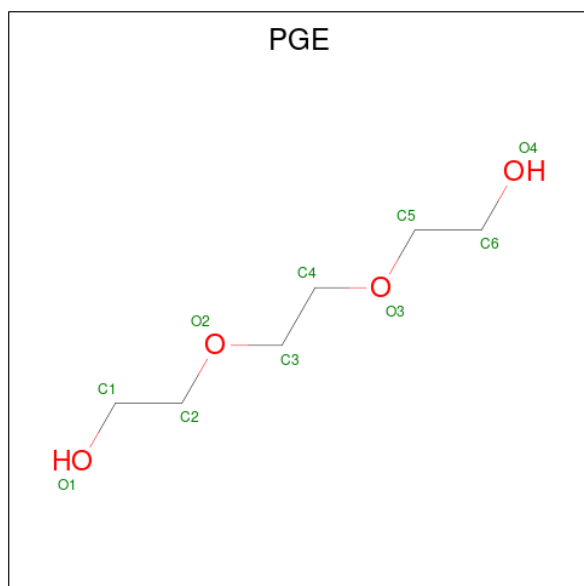
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	966	MSE	-	initiating methionine	UNP Q02630
E	966	MSE	-	initiating methionine	UNP Q02630
H	966	MSE	-	expression tag	UNP Q02630
K	966	MSE	-	initiating methionine	UNP Q02630

- Molecule 3 is a protein called Nucleoporin NUP159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	Se	0	0	0
			204	133	34	35	2			
3	F	26	Total	C	N	O	Se	0	0	0
			204	133	34	35	2			
3	I	28	Total	C	N	O	Se	0	0	0
			222	145	37	38	2			
3	L	24	Total	C	N	O	Se	0	0	0
			192	126	32	33	1			

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

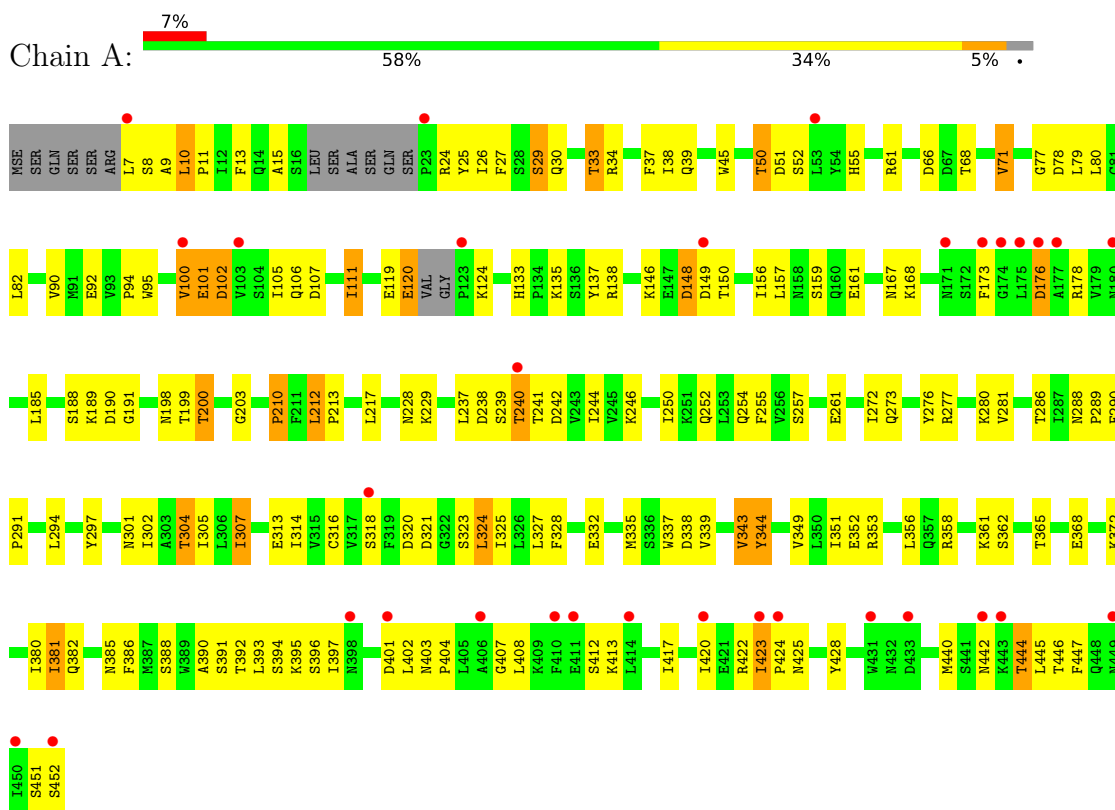


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	6	4		

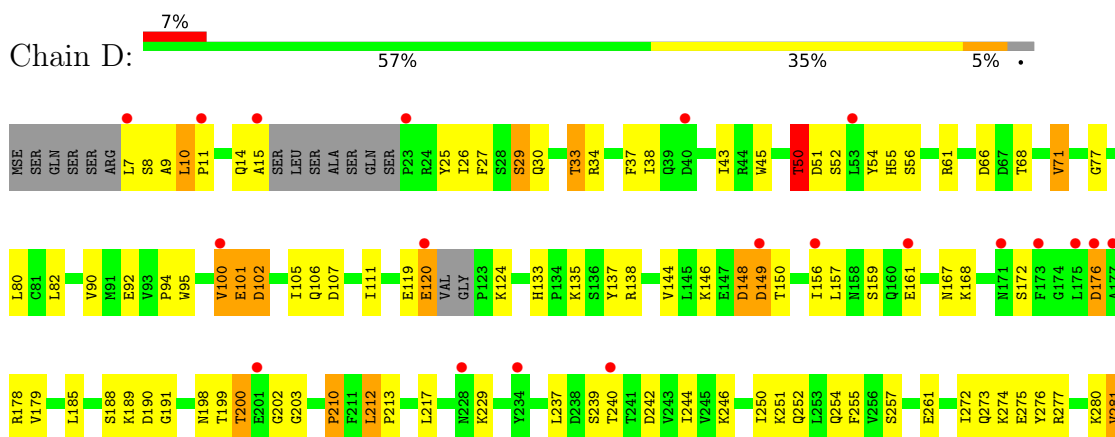
3 Residue-property plots

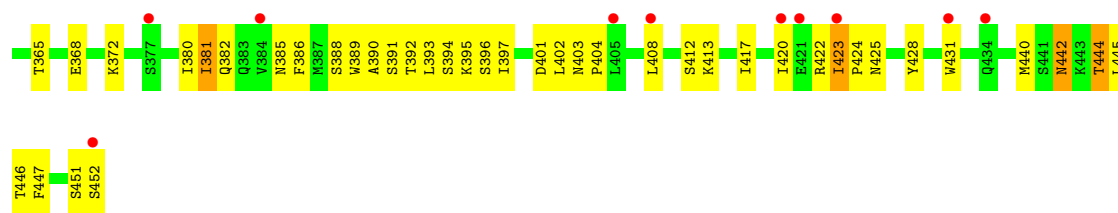
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Nucleoporin NUP82

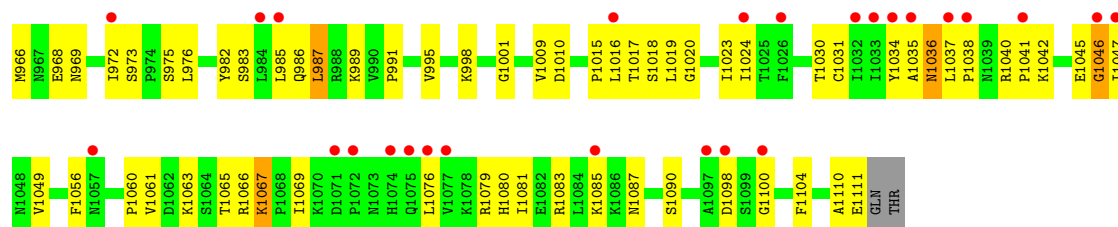


• Molecule 1: Nucleoporin NUP82

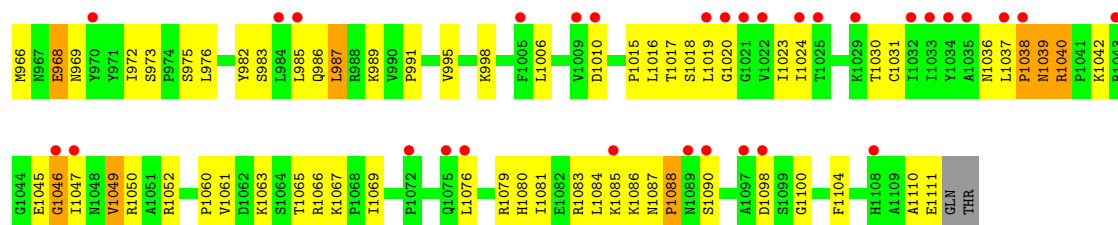




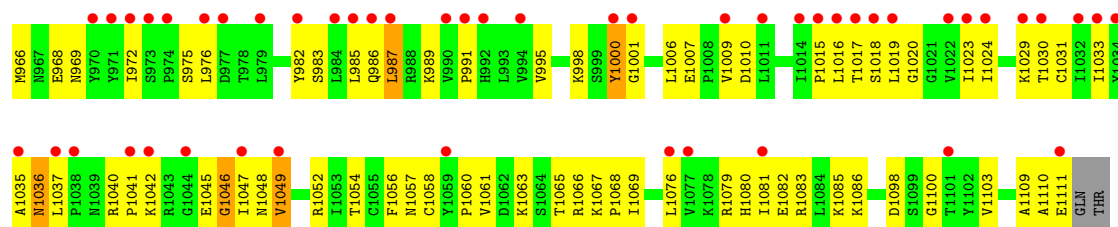
• Molecule 2: Nucleoporin NUP116/NSP116



• Molecule 2: Nucleoporin NUP116/NSP116

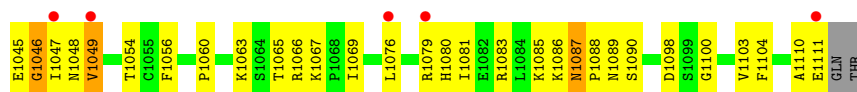


• Molecule 2: Nucleoporin NUP116/NSP116

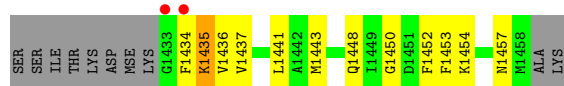


• Molecule 2: Nucleoporin NUP116/NSP116

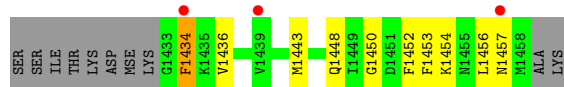
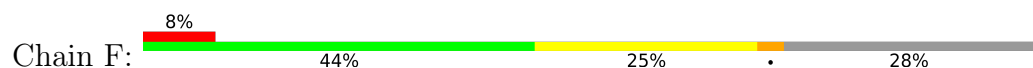




- Molecule 3: Nucleoporin NUP159



- Molecule 3: Nucleoporin NUP159



- Molecule 3: Nucleoporin NUP159



- Molecule 3: Nucleoporin NUP159



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 96.77Å 144.28Å 105.98° 93.97° 108.24°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 93.3 (50.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.257 , 0.272 0.238 , 0.265	Depositor DCC
R_{free} test set	6890 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.889	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19653	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PGE

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	0.49	0/3603	1.00	14/4877 (0.3%)
1	D	0.49	0/3597	0.99	10/4869 (0.2%)
1	G	0.48	0/3603	0.99	8/4877 (0.2%)
1	J	0.49	0/3614	1.00	13/4891 (0.3%)
2	B	0.43	0/1193	1.02	8/1617 (0.5%)
2	E	0.44	0/1193	1.01	5/1617 (0.3%)
2	H	0.46	0/1193	0.98	5/1617 (0.3%)
2	K	0.43	0/1193	0.98	5/1617 (0.3%)
3	C	0.58	0/204	1.01	0/266
3	F	0.54	0/204	0.97	0/266
3	I	0.46	0/222	1.08	2/288 (0.7%)
3	L	0.47	0/193	0.83	0/254
All	All	0.48	0/20012	1.00	70/27056 (0.3%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1039	ASN	N-CA-C	-8.91	102.97	113.21
1	G	52	SER	N-CA-C	-7.93	104.08	114.31
1	A	52	SER	N-CA-C	-7.84	104.20	114.31
1	D	52	SER	N-CA-C	-7.71	104.36	114.31
1	J	52	SER	N-CA-C	-7.65	104.45	114.31
1	J	343	VAL	N-CA-C	-7.62	96.38	108.95
2	E	987	LEU	N-CA-C	-7.41	104.27	112.72
2	B	987	LEU	N-CA-C	-7.37	104.32	112.72
2	H	987	LEU	N-CA-C	-7.30	104.40	112.72
1	G	343	VAL	N-CA-C	-7.19	97.09	108.95
1	D	343	VAL	N-CA-C	-7.10	97.23	108.95
2	K	1100	GLY	N-CA-C	-7.05	105.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	VAL	N-CA-C	-7.02	97.36	108.95
3	I	1434	PHE	CA-C-N	-6.96	109.73	120.31
3	I	1434	PHE	C-N-CA	-6.96	109.73	120.31
2	H	1100	GLY	N-CA-C	-6.95	105.64	115.30
2	B	1100	GLY	N-CA-C	-6.92	105.68	115.30
1	J	176	ASP	N-CA-C	6.91	120.92	111.39
2	H	976	LEU	N-CA-C	-6.85	104.19	112.54
2	E	1100	GLY	N-CA-C	-6.79	105.86	115.30
2	K	987	LEU	N-CA-C	-6.76	105.01	112.72
1	D	176	ASP	N-CA-C	6.75	120.70	111.39
1	G	176	ASP	N-CA-C	6.74	120.68	111.39
1	G	212	LEU	N-CA-C	6.64	119.02	110.39
1	J	212	LEU	N-CA-C	6.63	119.01	110.39
2	E	976	LEU	N-CA-C	-6.58	104.52	112.54
1	A	176	ASP	N-CA-C	6.57	120.46	111.39
1	A	212	LEU	N-CA-C	6.49	118.83	110.39
1	D	212	LEU	N-CA-C	6.44	118.77	110.39
2	B	976	LEU	N-CA-C	-6.39	104.75	112.54
2	K	976	LEU	N-CA-C	-6.33	104.82	112.54
1	D	239	SER	N-CA-C	5.89	118.65	111.82
1	A	381	ILE	N-CA-C	-5.87	97.38	107.24
1	D	381	ILE	N-CA-C	-5.81	97.48	107.24
2	H	1063	LYS	N-CA-C	5.70	119.33	112.38
1	D	149	ASP	N-CA-C	-5.68	101.71	113.31
2	B	1037	LEU	CA-C-N	5.68	125.61	119.76
2	B	1037	LEU	C-N-CA	5.68	125.61	119.76
1	D	50	THR	N-CA-C	5.68	120.70	113.55
1	J	381	ILE	N-CA-C	-5.64	97.77	107.24
2	B	1063	LYS	N-CA-C	5.52	119.12	112.38
1	A	240	THR	N-CA-C	-5.49	105.45	111.82
1	A	50	THR	N-CA-C	5.49	120.46	113.55
2	K	1063	LYS	N-CA-C	5.48	119.07	112.38
1	G	381	ILE	N-CA-C	-5.47	98.05	107.24
1	A	444	THR	N-CA-C	5.43	116.89	109.18
1	G	50	THR	N-CA-C	5.42	120.37	113.55
2	H	1000	TYR	N-CA-C	5.41	119.89	113.12
1	G	313	GLU	N-CA-C	5.38	117.16	109.14
1	D	313	GLU	N-CA-C	5.37	117.14	109.14
2	E	1063	LYS	N-CA-C	5.36	118.92	112.38
1	J	346	ASN	N-CA-C	-5.36	101.58	109.62
1	A	313	GLU	N-CA-C	5.33	117.08	109.14
1	J	444	THR	N-CA-C	5.27	116.66	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LEU	CA-C-N	5.23	126.38	119.84
1	A	10	LEU	C-N-CA	5.23	126.38	119.84
1	J	50	THR	N-CA-C	5.22	120.13	113.55
2	B	1067	LYS	CA-C-N	5.20	125.36	119.90
2	B	1067	LYS	C-N-CA	5.20	125.36	119.90
2	K	1000	TYR	N-CA-C	5.18	119.60	113.12
1	A	13	PHE	N-CA-C	5.15	118.02	111.69
1	J	313	GLU	N-CA-C	5.13	116.78	109.14
1	J	140	SER	N-CA-C	5.12	119.25	113.15
1	A	173	PHE	N-CA-C	-5.11	101.64	109.41
1	J	239	SER	N-CA-C	-5.10	107.03	114.12
1	G	444	THR	N-CA-C	5.09	116.41	109.18
1	J	74	SER	N-CA-C	-5.08	103.34	110.50
1	J	133	HIS	N-CA-C	-5.07	101.91	109.42
1	A	111	ILE	N-CA-C	5.01	119.42	112.35
1	D	144	VAL	N-CA-C	5.00	115.05	107.75

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	3539	0	3507	148	0
1	D	3533	0	3502	158	0
1	G	3539	0	3507	161	0
1	J	3550	0	3520	161	0
2	B	1165	0	1183	41	0
2	E	1165	0	1183	48	0
2	H	1165	0	1183	56	0
2	K	1165	0	1183	49	0
3	C	204	0	213	11	0
3	F	204	0	213	12	0
3	I	222	0	237	13	0
3	L	192	0	201	10	0
4	D	10	0	14	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19653	0	19646	823	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 21.

All (823) 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:H:1010:ASP:HB3	2:H:1046:GLY:HA2	1.41	0.99
1:G:10:LEU:HD12	1:G:11:PRO:HD2	1.51	0.92
1:J:444:THR:HG22	1:J:445:LEU:H	1.40	0.86
3:I:1437:VAL:HG11	1:J:243:VAL:HG12	1.58	0.85
1:G:444:THR:HG22	1:G:445:LEU:H	1.40	0.84
1:A:210:PRO:HG3	1:A:335:MSE:HE3	1.60	0.83
1:G:210:PRO:HG3	1:G:335:MSE:HE3	1.59	0.82
1:D:92:GLU:HB2	1:D:111:ILE:HD11	1.62	0.82
1:A:10:LEU:HD12	1:A:11:PRO:HD2	1.59	0.82
1:D:444:THR:HG22	1:D:445:LEU:H	1.41	0.81
1:J:90:VAL:HG11	1:J:156:ILE:HD13	1.62	0.81
1:A:210:PRO:CG	1:A:335:MSE:HE3	2.10	0.81
2:B:983:SER:HB2	2:B:986:GLN:HG2	1.63	0.81
2:E:1038:PRO:C	2:E:1040:ARG:H	1.85	0.81
2:E:983:SER:HB2	2:E:986:GLN:HG2	1.64	0.80
1:G:210:PRO:CG	1:G:335:MSE:HE3	2.12	0.80
2:H:983:SER:HB2	2:H:986:GLN:HG2	1.64	0.80
1:G:90:VAL:HG11	1:G:156:ILE:HD13	1.62	0.80
1:A:92:GLU:HB2	1:A:111:ILE:HD11	1.64	0.79
1:D:148:ASP:HB3	1:D:150:THR:HB	1.64	0.79
1:A:444:THR:HG22	1:A:445:LEU:H	1.43	0.79
1:J:381:ILE:HD11	1:J:424:PRO:HG3	1.65	0.79
2:H:1001:GLY:HA2	2:H:1056:PHE:CE2	2.17	0.79
1:A:148:ASP:HB3	1:A:150:THR:HB	1.64	0.78
1:D:343:VAL:HG11	2:E:1066:ARG:NH1	1.98	0.78
1:A:90:VAL:HG11	1:A:156:ILE:HD13	1.65	0.78
1:D:90:VAL:HG11	1:D:156:ILE:HD13	1.64	0.78
1:D:210:PRO:CG	1:D:335:MSE:HE3	2.13	0.78
1:D:210:PRO:HG3	1:D:335:MSE:HE3	1.65	0.77
1:J:343:VAL:HG11	2:K:1066:ARG:NH1	1.99	0.77
1:J:210:PRO:HG3	1:J:335:MSE:HE3	1.66	0.77
2:K:983:SER:HB2	2:K:986:GLN:HG2	1.65	0.77
2:H:972:ILE:HD11	2:H:1019:LEU:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ILE:HD11	1:D:424:PRO:HG3	1.66	0.77
1:J:210:PRO:CG	1:J:335:MSE:HE3	2.15	0.77
1:J:92:GLU:HB2	1:J:111:ILE:HD11	1.65	0.76
1:G:148:ASP:HB3	1:G:150:THR:HB	1.66	0.76
1:G:381:ILE:HD11	1:G:424:PRO:HG3	1.67	0.76
1:A:280:LYS:HD2	1:A:338:ASP:O	1.85	0.76
3:I:1441:LEU:HD11	1:J:243:VAL:HG13	1.68	0.76
1:D:358:ARG:CZ	1:D:380:ILE:HD12	2.17	0.75
1:J:148:ASP:HB3	1:J:150:THR:HB	1.67	0.75
1:J:358:ARG:CZ	1:J:380:ILE:HD12	2.16	0.75
1:J:392:THR:HG21	1:J:408:LEU:HD11	1.67	0.75
1:G:358:ARG:CZ	1:G:380:ILE:HD12	2.16	0.74
2:B:972:ILE:HD11	2:B:1019:LEU:HB2	1.69	0.74
1:G:92:GLU:HB2	1:G:111:ILE:HD11	1.67	0.74
1:G:255:PHE:CD2	1:G:335:MSE:HE1	2.22	0.74
1:G:280:LYS:HD2	1:G:338:ASP:O	1.87	0.74
1:J:361:LYS:HE2	1:J:423:ILE:HD11	1.69	0.74
1:D:289:PRO:HG3	3:F:1457:ASN:HB2	1.69	0.74
1:G:119:GLU:O	1:G:124:LYS:HE2	1.88	0.74
1:D:27:PHE:HZ	1:D:71:VAL:HG23	1.53	0.73
1:J:119:GLU:O	1:J:124:LYS:HE2	1.88	0.73
1:A:358:ARG:CZ	1:A:380:ILE:HD12	2.19	0.73
1:A:381:ILE:HD11	1:A:424:PRO:HG3	1.68	0.73
1:D:189:LYS:HG2	1:D:304:THR:CG2	2.19	0.73
1:D:392:THR:HG21	1:D:408:LEU:HD11	1.70	0.73
1:A:361:LYS:HE2	1:A:423:ILE:HD11	1.70	0.73
1:D:280:LYS:HD2	1:D:338:ASP:O	1.87	0.73
1:J:343:VAL:HG11	2:K:1066:ARG:CZ	2.19	0.73
1:D:66:ASP:OD1	1:D:68:THR:HB	1.88	0.73
1:A:392:THR:HG21	1:A:408:LEU:HD11	1.72	0.72
1:J:66:ASP:OD1	1:J:68:THR:HB	1.89	0.72
1:J:335:MSE:HE2	1:J:337:TRP:CZ2	2.25	0.72
2:K:1086:LYS:O	2:K:1087:ASN:HB3	1.88	0.72
2:K:972:ILE:HD11	2:K:1019:LEU:HB2	1.69	0.72
1:A:66:ASP:OD1	1:A:68:THR:HB	1.89	0.72
1:G:66:ASP:OD1	1:G:68:THR:HB	1.90	0.72
1:G:189:LYS:HG2	1:G:304:THR:CG2	2.19	0.72
1:J:37:PHE:HE1	1:J:440:MSE:HE1	1.54	0.72
1:D:335:MSE:HE2	1:D:337:TRP:CZ2	2.23	0.72
1:D:444:THR:HG22	1:D:445:LEU:N	2.04	0.72
1:A:119:GLU:O	1:A:124:LYS:HE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:MSE:HE2	1:A:337:TRP:CZ2	2.24	0.72
1:J:255:PHE:CD2	1:J:335:MSE:HE1	2.25	0.72
1:J:444:THR:HG22	1:J:445:LEU:N	2.05	0.72
2:E:972:ILE:HD11	2:E:1019:LEU:HB2	1.70	0.71
1:G:392:THR:HG21	1:G:408:LEU:HD11	1.72	0.71
1:G:361:LYS:HE2	1:G:423:ILE:HD11	1.72	0.71
1:G:444:THR:HG22	1:G:445:LEU:N	2.05	0.71
1:D:119:GLU:O	1:D:124:LYS:HE2	1.90	0.71
1:J:280:LYS:HD2	1:J:338:ASP:O	1.89	0.71
2:K:1090:SER:HB2	2:K:1104:PHE:CD2	2.25	0.71
1:A:27:PHE:HZ	1:A:71:VAL:HG23	1.55	0.70
3:C:1434:PHE:O	3:C:1436:VAL:N	2.24	0.70
1:J:27:PHE:HZ	1:J:71:VAL:HG23	1.54	0.70
1:J:237:LEU:HD22	1:J:246:LYS:HG3	1.73	0.70
1:G:27:PHE:HZ	1:G:71:VAL:HG23	1.55	0.70
1:G:173:PHE:HE2	2:H:1033:ILE:HD12	1.56	0.70
1:A:444:THR:HG22	1:A:445:LEU:N	2.06	0.70
1:D:255:PHE:CD2	1:D:335:MSE:HE1	2.26	0.70
1:G:335:MSE:HE2	1:G:337:TRP:CZ2	2.27	0.69
1:A:189:LYS:HG2	1:A:304:THR:CG2	2.22	0.69
1:G:7:LEU:HB2	1:G:431:TRP:CZ3	2.27	0.69
1:A:255:PHE:CD2	1:A:335:MSE:HE1	2.26	0.69
1:D:34:ARG:HB3	1:D:95:TRP:CH2	2.28	0.69
1:D:361:LYS:HE2	1:D:423:ILE:HD11	1.74	0.69
1:D:440:MSE:HE2	1:D:445:LEU:HD13	1.75	0.69
2:K:1010:ASP:HB3	2:K:1046:GLY:HA2	1.75	0.69
2:H:989:LYS:O	2:H:991:PRO:HD3	1.94	0.68
1:J:325:ILE:HD12	1:J:327:LEU:HD21	1.75	0.68
2:E:989:LYS:O	2:E:991:PRO:HD3	1.94	0.67
2:H:1042:LYS:O	2:H:1045:GLU:HB2	1.95	0.67
1:G:343:VAL:HG11	2:H:1066:ARG:NH1	2.10	0.67
2:K:989:LYS:O	2:K:991:PRO:HD3	1.94	0.67
2:B:989:LYS:O	2:B:991:PRO:HD3	1.95	0.66
2:K:1037:LEU:N	2:K:1038:PRO:HD3	2.09	0.66
2:B:1042:LYS:O	2:B:1045:GLU:HB2	1.95	0.66
1:A:15:ALA:HB2	1:A:24:ARG:HH21	1.61	0.66
1:D:301:ASN:H	1:D:318:SER:HB2	1.61	0.66
1:J:422:ARG:HG3	1:J:442:ASN:HD21	1.58	0.66
3:I:1437:VAL:CG1	1:J:243:VAL:HG12	2.25	0.66
1:A:325:ILE:HD12	1:A:327:LEU:HD21	1.78	0.66
1:A:440:MSE:HE2	1:A:445:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:335:MSE:HE2	1:J:337:TRP:CH2	2.31	0.65
1:A:422:ARG:HG3	1:A:442:ASN:HD21	1.61	0.65
1:D:422:ARG:HG3	1:D:442:ASN:HD21	1.61	0.65
2:H:1010:ASP:HB3	2:H:1046:GLY:CA	2.21	0.65
1:J:189:LYS:HG2	1:J:304:THR:CG2	2.26	0.65
1:J:440:MSE:HE2	1:J:445:LEU:HD13	1.76	0.65
1:D:343:VAL:HG11	2:E:1066:ARG:CZ	2.26	0.65
1:G:440:MSE:HE2	1:G:445:LEU:HD13	1.78	0.65
1:D:30:GLN:O	1:D:33:THR:HB	1.97	0.65
2:H:1082:GLU:HG2	2:H:1086:LYS:HE3	1.79	0.65
1:J:30:GLN:O	1:J:33:THR:HB	1.96	0.65
1:A:92:GLU:HB2	1:A:111:ILE:CD1	2.26	0.64
1:J:34:ARG:HB3	1:J:95:TRP:CH2	2.31	0.64
1:J:92:GLU:HB2	1:J:111:ILE:CD1	2.26	0.64
1:G:34:ARG:HB3	1:G:95:TRP:CH2	2.32	0.64
1:G:255:PHE:CE2	1:G:335:MSE:HE1	2.32	0.64
1:A:301:ASN:H	1:A:318:SER:HB2	1.63	0.64
1:G:335:MSE:HE2	1:G:337:TRP:CH2	2.32	0.64
1:G:422:ARG:HG3	1:G:442:ASN:HD21	1.61	0.64
1:J:307:ILE:HD11	1:J:314:ILE:HD11	1.78	0.64
2:B:1090:SER:HB2	2:B:1104:PHE:CD2	2.33	0.64
1:G:30:GLN:O	1:G:33:THR:HB	1.97	0.64
2:K:1042:LYS:O	2:K:1045:GLU:HB2	1.97	0.64
2:K:1069:ILE:HD12	2:K:1076:LEU:HD12	1.80	0.64
1:A:30:GLN:O	1:A:33:THR:HB	1.98	0.64
1:A:34:ARG:HB3	1:A:95:TRP:CH2	2.33	0.64
2:E:1042:LYS:O	2:E:1045:GLU:HB2	1.97	0.64
1:D:25:TYR:CD2	1:D:71:VAL:HG22	2.33	0.63
1:D:92:GLU:HB2	1:D:111:ILE:CD1	2.26	0.63
1:G:25:TYR:CD2	1:G:71:VAL:HG22	2.34	0.63
1:J:255:PHE:CE2	1:J:335:MSE:HE1	2.34	0.63
1:G:92:GLU:HB2	1:G:111:ILE:CD1	2.28	0.63
1:J:301:ASN:H	1:J:318:SER:HB2	1.64	0.63
1:G:29:SER:OG	1:G:77:GLY:HA3	1.98	0.63
1:A:335:MSE:HE2	1:A:337:TRP:CH2	2.34	0.62
1:D:335:MSE:HE2	1:D:337:TRP:CH2	2.33	0.62
1:G:301:ASN:H	1:G:318:SER:HB2	1.63	0.62
2:B:1015:PRO:HG2	2:B:1018:SER:OG	1.99	0.62
1:D:26:ILE:HB	1:D:440:MSE:HE3	1.80	0.62
1:D:255:PHE:CE2	1:D:335:MSE:HE1	2.34	0.62
1:G:380:ILE:HG22	1:G:381:ILE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:PHE:HE1	1:J:440:MSE:CE	2.12	0.62
1:J:402:LEU:HD21	3:L:1448:GLN:HB3	1.79	0.62
1:G:100:VAL:HG12	1:G:106:GLN:HG2	1.82	0.62
2:E:1069:ILE:HD12	2:E:1076:LEU:HD12	1.82	0.62
1:G:307:ILE:HD11	1:G:314:ILE:HD11	1.80	0.62
1:A:25:TYR:CD2	1:A:71:VAL:HG22	2.34	0.62
1:J:444:THR:CG2	1:J:445:LEU:H	2.13	0.62
2:E:1015:PRO:HG2	2:E:1018:SER:OG	2.00	0.62
2:H:1015:PRO:HG2	2:H:1018:SER:OG	2.00	0.62
1:A:372:LYS:HE2	1:A:385:ASN:ND2	2.16	0.61
2:E:1038:PRO:C	2:E:1040:ARG:N	2.57	0.61
1:A:255:PHE:CE2	1:A:335:MSE:HE1	2.35	0.61
1:D:100:VAL:HG12	1:D:106:GLN:HG2	1.80	0.61
1:D:380:ILE:HG22	1:D:381:ILE:N	2.14	0.61
1:A:38:ILE:HD11	1:A:80:LEU:HD13	1.83	0.61
1:A:146:LYS:HB2	1:A:150:THR:HG22	1.82	0.61
2:B:1069:ILE:HD12	2:B:1076:LEU:HD12	1.82	0.61
2:H:1069:ILE:HD12	2:H:1076:LEU:HD12	1.81	0.61
2:K:1015:PRO:HG2	2:K:1018:SER:OG	1.99	0.61
3:C:1434:PHE:C	3:C:1436:VAL:H	2.08	0.61
1:A:148:ASP:O	1:A:149:ASP:HB2	2.00	0.61
1:D:372:LYS:HE2	1:D:385:ASN:ND2	2.16	0.61
1:J:380:ILE:HG22	1:J:381:ILE:N	2.15	0.61
1:A:380:ILE:HG22	1:A:381:ILE:N	2.14	0.61
1:D:146:LYS:HB2	1:D:150:THR:HG22	1.81	0.61
1:D:297:TYR:HB3	1:D:320:ASP:HB2	1.83	0.61
1:J:100:VAL:HG12	1:J:106:GLN:HG2	1.83	0.61
2:B:1040:ARG:N	2:B:1041:PRO:HD3	2.15	0.61
1:D:307:ILE:HD11	1:D:314:ILE:HD11	1.83	0.61
1:G:148:ASP:O	1:G:149:ASP:HB2	2.00	0.61
1:A:343:VAL:O	1:A:344:TYR:HB2	2.01	0.60
1:D:38:ILE:HD11	1:D:80:LEU:HD13	1.84	0.60
1:D:148:ASP:O	1:D:149:ASP:HB2	2.00	0.60
1:A:307:ILE:HD11	1:A:314:ILE:HD11	1.84	0.60
1:G:444:THR:CG2	1:G:445:LEU:H	2.13	0.60
2:K:1081:ILE:HG22	2:K:1085:LYS:HE3	1.84	0.60
1:J:148:ASP:O	1:J:149:ASP:HB2	2.02	0.60
1:J:25:TYR:CD2	1:J:71:VAL:HG22	2.37	0.60
1:A:297:TYR:HB3	1:A:320:ASP:HB2	1.84	0.60
1:G:38:ILE:HD11	1:G:80:LEU:HD13	1.84	0.60
1:G:146:LYS:HB2	1:G:150:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:372:LYS:HE2	1:J:385:ASN:ND2	2.16	0.59
2:K:1065:THR:HG22	2:K:1067:LYS:HG3	1.83	0.59
1:D:325:ILE:HD12	1:D:327:LEU:HD21	1.84	0.59
1:G:325:ILE:HD12	1:G:327:LEU:HD21	1.84	0.59
1:G:10:LEU:HD21	1:G:46:TYR:CE2	2.37	0.59
1:G:343:VAL:O	1:G:344:TYR:HB2	2.03	0.59
1:J:82:LEU:HD12	1:J:82:LEU:N	2.17	0.59
1:A:100:VAL:HG12	1:A:106:GLN:HG2	1.83	0.59
1:D:343:VAL:O	1:D:344:TYR:HB2	2.02	0.59
2:H:1110:ALA:O	2:H:1111:GLU:HG3	2.03	0.59
2:K:969:ASN:O	2:K:998:LYS:HG3	2.03	0.59
1:G:37:PHE:HE1	1:G:440:MSE:HE1	1.68	0.58
1:J:297:TYR:HB3	1:J:320:ASP:HB2	1.84	0.58
2:H:1081:ILE:HG22	2:H:1085:LYS:HE3	1.85	0.58
1:A:343:VAL:HG11	2:B:1066:ARG:NH1	2.18	0.58
2:H:1029:LYS:HE2	2:H:1057:ASN:O	2.03	0.58
1:G:372:LYS:HE2	1:G:385:ASN:ND2	2.17	0.58
1:A:289:PRO:HG3	3:C:1457:ASN:HB2	1.85	0.58
1:J:386:PHE:HB3	1:J:412:SER:OG	2.03	0.58
2:B:1110:ALA:O	2:B:1111:GLU:HG3	2.04	0.58
1:A:305:ILE:HD12	1:A:305:ILE:N	2.19	0.58
1:D:349:VAL:HG11	3:F:1453:PHE:HB2	1.85	0.58
1:G:386:PHE:HB3	1:G:412:SER:OG	2.04	0.58
2:E:1065:THR:HG22	2:E:1067:LYS:HG3	1.84	0.57
1:G:26:ILE:HB	1:G:440:MSE:HE3	1.86	0.57
1:D:402:LEU:HD21	3:F:1448:GLN:HB3	1.84	0.57
1:D:444:THR:CG2	1:D:445:LEU:H	2.14	0.57
1:G:305:ILE:N	1:G:305:ILE:HD12	2.19	0.57
3:I:1437:VAL:CG1	1:J:243:VAL:CG1	2.82	0.57
1:G:297:TYR:HB3	1:G:320:ASP:HB2	1.85	0.57
3:L:1452:PHE:CE1	3:L:1456:LEU:HD22	2.39	0.57
1:G:349:VAL:HG11	3:I:1453:PHE:HB2	1.86	0.57
1:A:444:THR:CG2	1:A:445:LEU:H	2.15	0.57
2:B:966:MSE:HG3	2:B:1020:GLY:HA3	1.86	0.57
2:H:1000:TYR:C	2:H:1056:PHE:CD2	2.83	0.57
1:J:307:ILE:HD11	1:J:314:ILE:CD1	2.34	0.57
1:J:343:VAL:O	1:J:344:TYR:HB2	2.05	0.57
2:K:1110:ALA:O	2:K:1111:GLU:HG3	2.04	0.57
1:A:257:SER:O	1:A:261:GLU:HG3	2.04	0.57
2:B:1065:THR:HG22	2:B:1067:LYS:HG3	1.85	0.57
2:B:1081:ILE:HG22	2:B:1085:LYS:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:SER:OG	1:D:77:GLY:HA3	2.05	0.57
1:G:257:SER:O	1:G:261:GLU:HG3	2.05	0.57
2:B:983:SER:CB	2:B:986:GLN:HG2	2.35	0.56
2:H:1065:THR:HG22	2:H:1067:LYS:HG3	1.87	0.56
3:I:1456:LEU:HD12	3:I:1456:LEU:O	2.05	0.56
1:J:146:LYS:HB2	1:J:150:THR:HG22	1.87	0.56
1:J:440:MSE:CE	1:J:445:LEU:HD13	2.35	0.56
1:A:29:SER:OG	1:A:77:GLY:HA3	2.05	0.56
1:A:29:SER:HB3	1:A:34:ARG:HD3	1.87	0.56
2:E:983:SER:CB	2:E:986:GLN:HG2	2.35	0.56
2:H:966:MSE:HG3	2:H:1020:GLY:HA3	1.87	0.56
1:J:305:ILE:N	1:J:305:ILE:HD12	2.21	0.56
2:K:966:MSE:HG3	2:K:1020:GLY:HA3	1.86	0.56
2:K:1065:THR:HG21	2:K:1067:LYS:HD2	1.88	0.56
2:E:1065:THR:HG21	2:E:1067:LYS:HD2	1.86	0.56
2:H:1010:ASP:CB	2:H:1046:GLY:HA2	2.27	0.56
2:E:1081:ILE:HG22	2:E:1085:LYS:HE3	1.86	0.56
1:G:82:LEU:HD12	1:G:82:LEU:N	2.21	0.56
1:D:276:TYR:CE2	4:D:6119:PGE:H5	2.40	0.56
2:H:969:ASN:O	2:H:998:LYS:HG3	2.06	0.56
1:D:257:SER:O	1:D:261:GLU:HG3	2.05	0.56
1:D:422:ARG:O	1:D:423:ILE:C	2.49	0.56
1:J:242:ASP:OD1	1:J:244:ILE:N	2.39	0.56
2:E:1110:ALA:O	2:E:1111:GLU:HG3	2.06	0.56
1:J:38:ILE:HD11	1:J:80:LEU:HD13	1.88	0.56
1:G:29:SER:HB3	1:G:34:ARG:HD3	1.87	0.56
1:G:422:ARG:O	1:G:423:ILE:C	2.49	0.56
2:K:1087:ASN:C	2:K:1089:ASN:H	2.13	0.56
1:A:402:LEU:HD21	3:C:1448:GLN:HB3	1.88	0.55
1:D:242:ASP:OD1	1:D:244:ILE:N	2.39	0.55
1:J:29:SER:HB3	1:J:34:ARG:HD3	1.87	0.55
2:B:1010:ASP:HB3	2:B:1046:GLY:HA2	1.87	0.55
3:F:1434:PHE:CD1	3:F:1434:PHE:N	2.73	0.55
1:J:29:SER:OG	1:J:77:GLY:HA3	2.06	0.55
2:B:1065:THR:HG21	2:B:1067:LYS:HD2	1.87	0.55
2:B:969:ASN:O	2:B:998:LYS:HG3	2.06	0.55
2:E:969:ASN:O	2:E:998:LYS:HG3	2.05	0.55
2:H:983:SER:CB	2:H:986:GLN:HG2	2.35	0.55
1:A:386:PHE:HB3	1:A:412:SER:OG	2.06	0.55
2:K:1041:PRO:HB2	2:K:1048:ASN:HB2	1.88	0.55
2:H:1065:THR:HG21	2:H:1067:LYS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:HG11	2:B:1066:ARG:CZ	2.37	0.55
1:J:257:SER:O	1:J:261:GLU:HG3	2.07	0.55
1:J:381:ILE:HD11	1:J:420:ILE:HG21	1.89	0.55
1:A:422:ARG:O	1:A:423:ILE:C	2.50	0.54
2:E:966:MSE:HG3	2:E:1020:GLY:HA3	1.88	0.54
1:D:386:PHE:HB3	1:D:412:SER:OG	2.07	0.54
1:G:10:LEU:CD1	1:G:11:PRO:HD2	2.31	0.54
2:H:995:VAL:HG21	2:H:1024:ILE:HD12	1.88	0.54
1:A:210:PRO:HG3	1:A:335:MSE:CE	2.34	0.54
1:J:422:ARG:O	1:J:423:ILE:C	2.50	0.54
1:G:37:PHE:HE1	1:G:440:MSE:CE	2.21	0.54
1:J:189:LYS:NZ	1:J:304:THR:HG22	2.21	0.54
1:D:137:TYR:CE2	1:D:138:ARG:HG3	2.43	0.54
1:J:332:GLU:CB	3:L:1443:MSE:HE3	2.38	0.54
1:G:307:ILE:HD11	1:G:314:ILE:CD1	2.38	0.54
1:D:202:GLY:HA2	2:E:1079:ARG:HH12	1.72	0.54
1:G:210:PRO:HG3	1:G:335:MSE:CE	2.37	0.53
2:K:1001:GLY:HA2	2:K:1056:PHE:CE2	2.43	0.53
1:G:402:LEU:HD21	3:I:1448:GLN:HB3	1.91	0.53
1:J:402:LEU:HD21	3:L:1448:GLN:CB	2.38	0.53
1:G:332:GLU:CB	3:I:1443:MSE:HE3	2.39	0.53
2:K:1017:THR:HG22	2:K:1017:THR:O	2.08	0.53
1:A:349:VAL:HG11	3:C:1453:PHE:HB2	1.90	0.53
1:D:212:LEU:O	1:D:277:ARG:HD2	2.08	0.53
1:G:10:LEU:HD21	1:G:46:TYR:HE2	1.73	0.53
1:A:26:ILE:HB	1:A:440:MSE:HE3	1.90	0.53
2:H:982:TYR:HB2	2:H:987:LEU:HD13	1.90	0.53
1:A:242:ASP:OD1	1:A:244:ILE:N	2.42	0.53
1:D:7:LEU:HB2	1:D:431:TRP:CZ3	2.44	0.53
1:G:242:ASP:OD1	1:G:244:ILE:N	2.41	0.53
1:G:173:PHE:CZ	2:H:1109:ALA:O	2.62	0.53
1:A:82:LEU:N	1:A:82:LEU:HD12	2.24	0.53
1:A:138:ARG:NH2	1:A:157:LEU:HD13	2.24	0.53
1:A:380:ILE:CG2	1:A:381:ILE:N	2.71	0.53
1:D:9:ALA:O	1:D:10:LEU:C	2.52	0.53
1:G:199:THR:HG22	1:G:199:THR:O	2.09	0.53
1:D:307:ILE:HD11	1:D:314:ILE:CD1	2.39	0.52
1:J:229:LYS:HE3	1:J:332:GLU:CD	2.34	0.52
2:K:982:TYR:HB2	2:K:987:LEU:HD13	1.91	0.52
2:K:1009:VAL:HG13	2:K:1046:GLY:O	2.10	0.52
1:D:82:LEU:N	1:D:82:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:LEU:HD21	3:F:1448:GLN:CB	2.40	0.52
1:J:381:ILE:HD11	1:J:424:PRO:CG	2.38	0.52
1:D:305:ILE:HD12	1:D:305:ILE:N	2.24	0.52
1:D:380:ILE:CG2	1:D:381:ILE:N	2.72	0.52
1:G:380:ILE:CG2	1:G:381:ILE:N	2.72	0.52
1:J:289:PRO:HG3	3:L:1457:ASN:HB2	1.92	0.52
1:D:27:PHE:CZ	1:D:71:VAL:HG23	2.40	0.52
2:E:1037:LEU:N	2:E:1038:PRO:HD3	2.24	0.52
1:D:29:SER:HB3	1:D:34:ARG:HD3	1.90	0.52
2:B:1017:THR:O	2:B:1017:THR:HG22	2.10	0.52
1:J:356:LEU:O	1:J:358:ARG:HG3	2.10	0.52
3:I:1441:LEU:CD1	1:J:243:VAL:HG13	2.38	0.52
2:K:995:VAL:HG21	2:K:1024:ILE:HD12	1.91	0.52
1:D:138:ARG:NH2	1:D:157:LEU:HD13	2.25	0.52
1:A:307:ILE:HD11	1:A:314:ILE:CD1	2.40	0.51
1:G:381:ILE:HD11	1:G:420:ILE:HG21	1.92	0.51
1:J:138:ARG:NH2	1:J:157:LEU:HD13	2.25	0.51
1:J:422:ARG:CG	1:J:442:ASN:HD21	2.22	0.51
1:A:440:MSE:CE	1:A:445:LEU:HD13	2.39	0.51
1:G:138:ARG:NH2	1:G:157:LEU:HD13	2.25	0.51
1:A:240:THR:O	1:A:241:THR:C	2.54	0.51
1:D:440:MSE:CE	1:D:445:LEU:HD13	2.39	0.51
2:E:995:VAL:HG21	2:E:1024:ILE:HD12	1.92	0.51
1:J:393:LEU:O	1:J:397:ILE:HG13	2.10	0.51
2:K:983:SER:CB	2:K:986:GLN:HG2	2.35	0.51
1:D:393:LEU:O	1:D:397:ILE:HG13	2.11	0.51
1:D:403:ASN:HB2	1:D:404:PRO:HD3	1.93	0.51
1:G:27:PHE:CZ	1:G:71:VAL:HG23	2.42	0.51
1:G:30:GLN:CD	1:G:34:ARG:HD2	2.36	0.51
1:J:238:ASP:OD2	1:J:240:THR:HB	2.10	0.51
1:J:321:ASP:OD2	1:J:323:SER:HB2	2.09	0.51
1:A:420:ILE:HG21	1:A:424:PRO:HG3	1.93	0.51
1:J:349:VAL:HG11	3:L:1453:PHE:HB2	1.92	0.51
1:J:403:ASN:HB2	1:J:404:PRO:HD3	1.92	0.51
1:J:380:ILE:CG2	1:J:381:ILE:N	2.73	0.51
1:A:381:ILE:HD11	1:A:420:ILE:HG21	1.93	0.51
1:D:332:GLU:CB	3:F:1443:MSE:HE3	2.41	0.51
1:A:210:PRO:CB	1:A:335:MSE:HE3	2.40	0.51
2:H:1007:GLU:CD	2:H:1049:VAL:HG22	2.36	0.51
1:J:27:PHE:CZ	1:J:71:VAL:HG23	2.40	0.51
1:A:393:LEU:O	1:A:397:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ILE:HD11	1:D:420:ILE:HG21	1.92	0.50
2:E:1017:THR:O	2:E:1017:THR:HG22	2.11	0.50
1:G:238:ASP:OD2	1:G:240:THR:N	2.40	0.50
1:G:356:LEU:O	1:G:358:ARG:HG3	2.12	0.50
1:J:199:THR:O	1:J:199:THR:HG22	2.10	0.50
1:A:237:LEU:HD22	1:A:246:LYS:HG3	1.93	0.50
1:D:210:PRO:HG3	1:D:335:MSE:CE	2.39	0.50
2:H:1009:VAL:HG13	2:H:1046:GLY:O	2.10	0.50
1:J:137:TYR:CE2	1:J:138:ARG:HG3	2.46	0.50
1:A:388:SER:OG	1:A:413:LYS:HE3	2.11	0.50
3:L:1456:LEU:HG	3:L:1456:LEU:O	2.11	0.50
1:G:388:SER:OG	1:G:413:LYS:HE3	2.12	0.50
1:G:420:ILE:HG21	1:G:424:PRO:HG3	1.94	0.50
1:A:37:PHE:HE1	1:A:440:MSE:CE	2.25	0.50
2:B:1001:GLY:HA2	2:B:1056:PHE:CE2	2.47	0.50
2:H:1017:THR:HG22	2:H:1017:THR:O	2.12	0.50
1:J:210:PRO:CB	1:J:335:MSE:HE3	2.42	0.50
1:J:425:ASN:HB3	1:J:440:MSE:HB3	1.94	0.50
1:A:250:ILE:O	1:A:254:GLN:HG3	2.11	0.50
1:D:237:LEU:HD22	1:D:246:LYS:HG3	1.93	0.50
1:G:250:ILE:O	1:G:254:GLN:HG3	2.12	0.50
1:G:381:ILE:HD11	1:G:424:PRO:CG	2.38	0.50
1:A:199:THR:HG22	1:A:199:THR:O	2.10	0.50
1:A:403:ASN:HB2	1:A:404:PRO:HD3	1.94	0.50
1:G:7:LEU:HB2	1:G:431:TRP:CH2	2.46	0.50
1:J:7:LEU:C	1:J:9:ALA:H	2.20	0.50
1:A:446:THR:HG22	1:A:447:PHE:N	2.26	0.49
1:J:321:ASP:CG	1:J:323:SER:HB2	2.37	0.49
1:J:325:ILE:HG13	1:J:325:ILE:O	2.12	0.49
1:G:167:ASN:O	1:G:178:ARG:NH1	2.43	0.49
1:A:356:LEU:O	1:A:358:ARG:HG3	2.12	0.49
1:D:33:THR:HG22	1:D:34:ARG:HG3	1.94	0.49
1:G:403:ASN:HB2	1:G:404:PRO:HD3	1.93	0.49
1:A:27:PHE:CZ	1:A:71:VAL:HG23	2.42	0.49
2:B:995:VAL:HG21	2:B:1024:ILE:HD12	1.93	0.49
1:G:440:MSE:CE	1:G:445:LEU:HD13	2.40	0.49
1:J:30:GLN:CD	1:J:34:ARG:HD2	2.38	0.49
1:A:343:VAL:O	1:A:344:TYR:CB	2.61	0.49
1:D:199:THR:HG22	1:D:199:THR:O	2.12	0.49
1:G:45:TRP:CZ2	1:G:94:PRO:HB2	2.47	0.49
1:A:332:GLU:CB	3:C:1443:MSE:HE3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASN:HB3	1:A:440:MSE:HB3	1.94	0.49
1:D:189:LYS:HG2	1:D:304:THR:HG21	1.91	0.49
1:D:212:LEU:HD13	1:D:272:ILE:HD13	1.95	0.49
1:D:356:LEU:O	1:D:358:ARG:HG3	2.13	0.49
2:E:1018:SER:HB3	2:E:1023:ILE:HG13	1.94	0.49
1:G:30:GLN:CG	1:G:34:ARG:HD2	2.42	0.49
1:G:240:THR:HG22	1:G:240:THR:O	2.12	0.49
1:G:425:ASN:HB3	1:G:440:MSE:HB3	1.94	0.49
1:D:250:ILE:O	1:D:254:GLN:HG3	2.12	0.49
1:G:189:LYS:HG2	1:G:304:THR:HG22	1.94	0.49
1:G:239:SER:C	1:G:241:THR:H	2.21	0.49
2:E:982:TYR:HB2	2:E:987:LEU:HD13	1.93	0.49
1:A:167:ASN:O	1:A:178:ARG:NH1	2.46	0.48
1:A:392:THR:CG2	1:A:408:LEU:HD11	2.43	0.48
2:B:982:TYR:HB2	2:B:987:LEU:HD13	1.93	0.48
1:D:45:TRP:CZ2	1:D:94:PRO:HB2	2.48	0.48
1:J:392:THR:CG2	1:J:408:LEU:HD11	2.41	0.48
1:A:444:THR:CG2	1:A:445:LEU:N	2.75	0.48
1:D:45:TRP:CE2	1:D:55:HIS:HB2	2.49	0.48
1:D:210:PRO:CB	1:D:335:MSE:HE3	2.43	0.48
1:J:30:GLN:CG	1:J:34:ARG:HD2	2.44	0.48
1:A:45:TRP:CZ2	1:A:94:PRO:HB2	2.48	0.48
1:A:189:LYS:HG2	1:A:304:THR:HG22	1.95	0.48
1:A:381:ILE:HD11	1:A:424:PRO:CG	2.39	0.48
1:D:189:LYS:HG2	1:D:304:THR:HG22	1.95	0.48
1:D:343:VAL:O	1:D:344:TYR:CB	2.62	0.48
1:D:422:ARG:CG	1:D:442:ASN:HD21	2.25	0.48
3:L:1453:PHE:O	3:L:1457:ASN:ND2	2.43	0.48
1:D:133:HIS:CE1	1:D:213:PRO:HD3	2.49	0.48
1:G:273:GLN:OE1	1:G:276:TYR:HE1	1.97	0.48
1:G:325:ILE:O	1:G:325:ILE:HG13	2.14	0.48
1:G:451:SER:O	1:G:452:SER:HB3	2.13	0.48
1:J:420:ILE:HG21	1:J:424:PRO:HG3	1.95	0.48
1:J:451:SER:O	1:J:452:SER:HB3	2.13	0.48
1:A:61:ARG:NH1	1:A:107:ASP:OD1	2.46	0.48
3:F:1456:LEU:O	3:F:1456:LEU:HG	2.14	0.48
1:G:229:LYS:HE3	1:G:332:GLU:CD	2.39	0.48
1:J:391:SER:O	1:J:395:LYS:HG3	2.14	0.48
1:D:420:ILE:HG21	1:D:424:PRO:HG3	1.96	0.48
1:D:446:THR:HG22	1:D:447:PHE:N	2.28	0.48
1:A:198:ASN:O	1:A:203:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:CG	1:A:442:ASN:HD21	2.26	0.48
1:D:381:ILE:HD11	1:D:424:PRO:CG	2.38	0.48
1:D:425:ASN:HB3	1:D:440:MSE:HB3	1.95	0.48
1:D:451:SER:O	1:D:452:SER:HB3	2.13	0.48
3:F:1452:PHE:CE1	3:F:1456:LEU:HD22	2.49	0.48
1:G:237:LEU:HD22	1:G:246:LYS:HG3	1.96	0.48
1:J:250:ILE:O	1:J:254:GLN:HG3	2.14	0.48
1:A:321:ASP:OD2	1:A:323:SER:HB2	2.14	0.48
1:J:189:LYS:HZ3	1:J:304:THR:HG22	1.79	0.47
2:B:1018:SER:HB3	2:B:1023:ILE:HG13	1.96	0.47
1:D:148:ASP:HB3	1:D:150:THR:CB	2.41	0.47
1:G:391:SER:O	1:G:395:LYS:HG3	2.15	0.47
1:J:361:LYS:O	1:J:362:SER:HB3	2.14	0.47
1:A:451:SER:O	1:A:452:SER:HB3	2.14	0.47
3:I:1437:VAL:HG12	1:J:243:VAL:CG1	2.45	0.47
1:D:199:THR:O	1:D:200:THR:C	2.56	0.47
1:G:30:GLN:HG3	1:G:34:ARG:HD2	1.97	0.47
1:G:33:THR:HG22	1:G:34:ARG:HG3	1.96	0.47
2:K:1060:PRO:HG3	2:K:1080:HIS:CG	2.49	0.47
3:L:1452:PHE:CD1	3:L:1452:PHE:C	2.92	0.47
1:G:396:SER:HB2	1:G:401:ASP:O	2.15	0.47
1:J:7:LEU:N	1:J:431:TRP:CZ3	2.82	0.47
1:J:159:SER:C	1:J:161:GLU:H	2.22	0.47
1:A:33:THR:HG22	1:A:34:ARG:HG3	1.96	0.47
1:A:37:PHE:HE1	1:A:440:MSE:HE1	1.78	0.47
1:A:396:SER:HB2	1:A:401:ASP:O	2.14	0.47
3:C:1452:PHE:CD1	3:C:1452:PHE:C	2.92	0.47
1:D:159:SER:C	1:D:161:GLU:H	2.23	0.47
1:G:137:TYR:CE2	1:G:138:ARG:HG3	2.49	0.47
1:G:328:PHE:HB2	1:G:351:ILE:HD11	1.97	0.47
1:G:393:LEU:O	1:G:397:ILE:HG13	2.14	0.47
1:J:446:THR:HG22	1:J:447:PHE:N	2.29	0.47
1:A:148:ASP:HB3	1:A:150:THR:CB	2.42	0.47
1:D:396:SER:HB2	1:D:401:ASP:O	2.15	0.47
1:J:167:ASN:O	1:J:178:ARG:NH1	2.46	0.47
1:J:199:THR:O	1:J:200:THR:C	2.58	0.47
1:J:37:PHE:CE1	1:J:440:MSE:HE1	2.43	0.47
1:D:37:PHE:HE1	1:D:440:MSE:CE	2.28	0.47
1:G:173:PHE:HZ	2:H:1109:ALA:O	1.97	0.47
2:H:1036:ASN:O	2:H:1037:LEU:HB2	2.13	0.47
1:D:388:SER:OG	1:D:413:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1434:PHE:C	3:F:1436:VAL:H	2.23	0.46
1:G:45:TRP:CE2	1:G:55:HIS:HB2	2.50	0.46
3:I:1452:PHE:C	3:I:1452:PHE:CD1	2.92	0.46
1:J:45:TRP:CZ2	1:J:94:PRO:HB2	2.50	0.46
1:J:380:ILE:CG2	1:J:382:GLN:HG3	2.45	0.46
1:A:422:ARG:O	1:A:424:PRO:N	2.48	0.46
1:D:198:ASN:O	1:D:203:GLY:HA2	2.15	0.46
3:F:1434:PHE:O	3:F:1436:VAL:N	2.49	0.46
1:G:343:VAL:HG11	2:H:1066:ARG:CZ	2.45	0.46
1:G:352:GLU:CG	1:G:353:ARG:N	2.78	0.46
1:G:422:ARG:CG	1:G:442:ASN:HD21	2.26	0.46
1:J:352:GLU:CG	1:J:353:ARG:N	2.78	0.46
2:K:1034:TYR:CE2	2:K:1041:PRO:HG2	2.51	0.46
1:D:9:ALA:O	1:D:10:LEU:O	2.33	0.46
1:G:198:ASN:O	1:G:203:GLY:HA2	2.15	0.46
1:G:343:VAL:O	1:G:344:TYR:CB	2.62	0.46
1:G:361:LYS:O	1:G:362:SER:HB3	2.15	0.46
1:J:45:TRP:CE2	1:J:55:HIS:HB2	2.50	0.46
1:G:212:LEU:HD13	1:G:272:ILE:HD13	1.98	0.46
2:H:1001:GLY:CA	2:H:1056:PHE:CE2	2.96	0.46
1:A:159:SER:C	1:A:161:GLU:H	2.24	0.46
1:D:321:ASP:OD2	1:D:323:SER:HB2	2.15	0.46
1:G:133:HIS:CE1	1:G:213:PRO:HD3	2.50	0.46
1:G:392:THR:CG2	1:G:408:LEU:HD11	2.44	0.46
1:A:380:ILE:CG2	1:A:382:GLN:HG3	2.45	0.46
2:E:1039:ASN:O	2:E:1040:ARG:C	2.58	0.46
2:H:1000:TYR:C	2:H:1056:PHE:HD2	2.22	0.46
2:B:972:ILE:HD11	2:B:1019:LEU:CB	2.43	0.46
1:G:61:ARG:NH1	1:G:107:ASP:OD1	2.49	0.46
1:D:50:THR:HG22	1:D:51:ASP:OD1	2.15	0.46
1:D:251:LYS:NZ	4:D:6119:PGE:O2	2.45	0.46
1:G:159:SER:C	1:G:161:GLU:H	2.22	0.46
2:H:1018:SER:HB3	2:H:1023:ILE:HG13	1.96	0.46
1:A:321:ASP:CG	1:A:323:SER:HB2	2.41	0.46
2:B:1060:PRO:HG3	2:B:1080:HIS:CG	2.50	0.46
1:D:273:GLN:OE1	1:D:276:TYR:HE1	1.98	0.46
1:D:352:GLU:CG	1:D:353:ARG:N	2.78	0.46
2:E:1084:LEU:C	2:E:1086:LYS:H	2.23	0.46
1:A:30:GLN:CD	1:A:34:ARG:HD2	2.40	0.46
1:D:289:PRO:HD2	1:D:350:LEU:HB3	1.98	0.46
2:E:1090:SER:HB3	2:E:1104:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:GLU:H	1:G:120:GLU:HG3	1.47	0.46
2:H:1040:ARG:N	2:H:1041:PRO:HD3	2.30	0.46
2:H:1060:PRO:HG3	2:H:1080:HIS:CG	2.51	0.46
2:K:1030:THR:HG22	2:K:1031:CYS:N	2.31	0.46
1:A:212:LEU:HD13	1:A:272:ILE:HD13	1.98	0.45
3:F:1452:PHE:CD1	3:F:1452:PHE:C	2.93	0.45
1:J:388:SER:OG	1:J:413:LYS:HE3	2.16	0.45
1:A:402:LEU:HD21	3:C:1448:GLN:CB	2.46	0.45
2:E:1087:ASN:HB3	2:E:1090:SER:HB2	1.99	0.45
1:G:446:THR:HG22	1:G:447:PHE:N	2.30	0.45
2:K:1087:ASN:O	2:K:1087:ASN:CG	2.60	0.45
1:D:380:ILE:CG2	1:D:382:GLN:HG3	2.47	0.45
1:D:422:ARG:O	1:D:424:PRO:N	2.50	0.45
1:J:210:PRO:HB3	1:J:335:MSE:HE3	1.97	0.45
2:K:1018:SER:HB3	2:K:1023:ILE:HG13	1.98	0.45
1:A:45:TRP:CE2	1:A:55:HIS:HB2	2.52	0.45
1:A:137:TYR:CE2	1:A:138:ARG:HG3	2.51	0.45
2:B:972:ILE:HG12	2:B:995:VAL:HG22	1.97	0.45
2:E:1030:THR:HG22	2:E:1031:CYS:N	2.32	0.45
1:G:422:ARG:O	1:G:424:PRO:N	2.49	0.45
1:J:273:GLN:OE1	1:J:276:TYR:HE1	1.99	0.45
1:A:135:LYS:HD2	1:A:191:GLY:HA3	1.98	0.45
1:G:307:ILE:CG2	1:G:394:SER:HB3	2.47	0.45
1:J:198:ASN:O	1:J:203:GLY:HA2	2.16	0.45
2:K:1015:PRO:O	2:K:1017:THR:N	2.50	0.45
1:A:325:ILE:O	1:A:325:ILE:HG13	2.15	0.45
1:G:321:ASP:CG	1:G:323:SER:HB2	2.41	0.45
2:H:1082:GLU:O	2:H:1086:LYS:HG3	2.17	0.45
1:J:30:GLN:HB2	1:J:33:THR:HG22	1.98	0.45
1:J:61:ARG:NH1	1:J:107:ASP:OD1	2.49	0.45
1:J:189:LYS:HG2	1:J:304:THR:HG21	1.95	0.45
1:A:352:GLU:CG	1:A:353:ARG:N	2.79	0.45
1:A:368:GLU:HG2	1:A:428:TYR:CE2	2.51	0.45
2:B:1040:ARG:N	2:B:1041:PRO:CD	2.80	0.45
1:G:173:PHE:CE2	2:H:1033:ILE:HD12	2.45	0.45
2:H:1041:PRO:HB2	2:H:1048:ASN:HB2	1.99	0.45
1:J:422:ARG:O	1:J:424:PRO:N	2.49	0.45
2:K:1037:LEU:H	2:K:1038:PRO:HD3	1.80	0.45
2:B:1038:PRO:C	2:B:1040:ARG:H	2.24	0.45
1:D:255:PHE:HB2	4:D:6119:PGE:H6	1.98	0.45
1:J:343:VAL:O	1:J:344:TYR:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1009:VAL:HG13	2:B:1046:GLY:O	2.17	0.45
1:D:321:ASP:CG	1:D:323:SER:HB2	2.42	0.45
1:D:361:LYS:O	1:D:362:SER:HB3	2.16	0.45
1:D:368:GLU:HG2	1:D:428:TYR:CE2	2.52	0.45
1:J:212:LEU:HD13	1:J:272:ILE:HD13	1.98	0.45
1:J:307:ILE:CG2	1:J:394:SER:HB3	2.47	0.45
1:A:15:ALA:HB2	1:A:24:ARG:NH2	2.31	0.45
1:A:238:ASP:O	1:A:246:LYS:NZ	2.50	0.45
1:A:307:ILE:HG12	1:A:390:ALA:HB1	1.98	0.45
1:D:202:GLY:HA2	2:E:1079:ARG:NH1	2.32	0.45
1:J:82:LEU:HD12	1:J:82:LEU:H	1.81	0.45
1:J:210:PRO:HG3	1:J:335:MSE:CE	2.42	0.45
1:J:396:SER:HB2	1:J:401:ASP:O	2.17	0.45
2:K:972:ILE:HG12	2:K:995:VAL:HG22	1.99	0.44
1:D:392:THR:CG2	1:D:408:LEU:HD11	2.42	0.44
1:G:189:LYS:HG2	1:G:304:THR:HG21	1.95	0.44
2:H:972:ILE:HD11	2:H:1019:LEU:CB	2.43	0.44
1:A:199:THR:O	1:A:200:THR:C	2.60	0.44
1:A:328:PHE:HB2	1:A:351:ILE:HD11	1.99	0.44
2:H:1029:LYS:HE2	2:H:1058:CYS:HA	2.00	0.44
2:H:1030:THR:HG22	2:H:1031:CYS:N	2.31	0.44
1:J:30:GLN:HG3	1:J:34:ARG:HD2	2.00	0.44
1:D:30:GLN:CG	1:D:34:ARG:HD2	2.47	0.44
1:J:199:THR:O	1:J:199:THR:CG2	2.64	0.44
2:K:1060:PRO:HG3	2:K:1080:HIS:CD2	2.53	0.44
1:D:307:ILE:CG2	1:D:394:SER:HB3	2.48	0.44
1:G:199:THR:O	1:G:200:THR:C	2.60	0.44
1:G:380:ILE:CG2	1:G:382:GLN:HG3	2.48	0.44
1:J:368:GLU:HG2	1:J:428:TYR:CE2	2.52	0.44
1:J:380:ILE:HG21	1:J:382:GLN:HG3	2.00	0.44
1:D:188:SER:HB3	1:D:190:ASP:OD1	2.18	0.44
1:G:148:ASP:HB3	1:G:150:THR:CB	2.43	0.44
1:G:288:ASN:O	1:G:349:VAL:HA	2.18	0.44
1:G:321:ASP:OD2	1:G:323:SER:HB2	2.16	0.44
1:A:229:LYS:HE3	1:A:332:GLU:CD	2.42	0.44
2:B:1034:TYR:CE2	2:B:1041:PRO:HG2	2.52	0.44
1:D:167:ASN:O	1:D:178:ARG:NH1	2.51	0.44
1:D:291:PRO:HB2	1:D:294:LEU:HD12	2.00	0.44
1:D:391:SER:O	1:D:395:LYS:HG3	2.17	0.44
2:K:1040:ARG:O	2:K:1041:PRO:C	2.61	0.44
1:A:78:ASP:O	1:A:79:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:HB3	1:A:335:MSE:HE3	1.99	0.44
1:A:273:GLN:OE1	1:A:276:TYR:HE1	2.00	0.44
3:C:1450:GLY:O	3:C:1454:LYS:HG3	2.18	0.44
1:D:102:ASP:HB3	1:D:105:ILE:H	1.82	0.44
1:D:251:LYS:HZ1	4:D:6119:PGE:C2	2.31	0.44
2:E:1049:VAL:HG13	2:E:1050:ARG:N	2.33	0.44
2:E:1060:PRO:HG3	2:E:1080:HIS:CG	2.52	0.44
1:G:368:GLU:HG2	1:G:428:TYR:CE2	2.52	0.44
1:A:199:THR:O	1:A:199:THR:CG2	2.65	0.43
1:D:30:GLN:HG3	1:D:34:ARG:HD2	2.00	0.43
1:D:61:ARG:NH1	1:D:107:ASP:OD1	2.49	0.43
1:J:102:ASP:HB3	1:J:105:ILE:H	1.83	0.43
1:A:30:GLN:CG	1:A:34:ARG:HD2	2.48	0.43
1:G:210:PRO:CB	1:G:335:MSE:HE3	2.48	0.43
2:K:1007:GLU:CD	2:K:1049:VAL:HG22	2.43	0.43
1:A:133:HIS:CE1	1:A:213:PRO:HD3	2.54	0.43
2:B:1030:THR:HG22	2:B:1031:CYS:N	2.33	0.43
1:D:358:ARG:NH2	1:D:380:ILE:HD12	2.33	0.43
1:A:381:ILE:O	1:A:417:ILE:HB	2.18	0.43
1:A:407:GLY:O	1:A:408:LEU:C	2.62	0.43
1:D:7:LEU:C	1:D:9:ALA:H	2.27	0.43
1:D:54:TYR:CD1	1:D:54:TYR:C	2.96	0.43
1:D:172:SER:HB3	2:E:1030:THR:HG23	1.98	0.43
2:K:1079:ARG:O	2:K:1083:ARG:HG2	2.19	0.43
1:A:189:LYS:HG2	1:A:304:THR:HG21	1.97	0.43
1:A:391:SER:O	1:A:395:LYS:HG3	2.18	0.43
1:G:289:PRO:HD2	1:G:350:LEU:HB3	2.00	0.43
2:H:1060:PRO:HG3	2:H:1080:HIS:CD2	2.53	0.43
1:J:133:HIS:CE1	1:J:213:PRO:HD3	2.54	0.43
1:J:307:ILE:HG12	1:J:390:ALA:HB1	2.01	0.43
1:A:361:LYS:O	1:A:362:SER:HB3	2.18	0.43
1:D:288:ASN:O	1:D:349:VAL:HA	2.19	0.43
1:G:199:THR:O	1:G:199:THR:CG2	2.65	0.43
1:G:381:ILE:O	1:G:417:ILE:HB	2.17	0.43
2:H:1047:ILE:HG22	2:H:1047:ILE:O	2.19	0.43
2:B:1015:PRO:O	2:B:1017:THR:N	2.51	0.43
2:B:1060:PRO:HG3	2:B:1080:HIS:CD2	2.54	0.43
1:J:291:PRO:HB2	1:J:294:LEU:HD12	2.00	0.43
2:E:968:GLU:H	2:E:968:GLU:HG3	1.45	0.43
1:G:15:ALA:O	1:G:16:SER:C	2.61	0.43
1:G:102:ASP:HB3	1:G:105:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:CYS:SG	1:A:324:LEU:HG	2.59	0.43
1:D:30:GLN:CD	1:D:34:ARG:HD2	2.43	0.43
2:H:1035:ALA:O	2:H:1036:ASN:C	2.61	0.43
1:J:119:GLU:O	1:J:120:GLU:C	2.62	0.43
1:J:247:ARG:NH1	1:J:338:ASP:OD2	2.49	0.43
2:K:1036:ASN:O	2:K:1037:LEU:HB2	2.19	0.43
2:K:1047:ILE:O	2:K:1047:ILE:HG22	2.19	0.43
1:A:380:ILE:HG21	1:A:382:GLN:HG3	2.00	0.43
1:D:213:PRO:O	1:D:277:ARG:HD3	2.18	0.43
1:G:168:LYS:O	1:G:178:ARG:HD3	2.19	0.43
2:H:1006:LEU:HD21	2:H:1052:ARG:NH1	2.34	0.43
2:H:1079:ARG:O	2:H:1083:ARG:HG2	2.18	0.43
1:J:328:PHE:HB2	1:J:351:ILE:HD11	2.01	0.43
1:J:386:PHE:HB2	1:J:389:TRP:CE2	2.54	0.43
1:A:307:ILE:CG2	1:A:394:SER:HB3	2.49	0.42
2:E:966:MSE:HE2	2:E:1020:GLY:CA	2.49	0.42
1:J:381:ILE:O	1:J:417:ILE:HB	2.18	0.42
1:A:102:ASP:HB3	1:A:105:ILE:H	1.84	0.42
1:A:212:LEU:O	1:A:277:ARG:HD2	2.18	0.42
1:A:321:ASP:OD2	1:A:353:ARG:NH2	2.52	0.42
2:B:1035:ALA:O	2:B:1036:ASN:C	2.62	0.42
1:D:10:LEU:HA	1:D:11:PRO:HD3	1.93	0.42
1:D:210:PRO:HB3	1:D:335:MSE:HE3	1.99	0.42
1:D:307:ILE:HG12	1:D:390:ALA:HB1	2.01	0.42
1:D:328:PHE:HB2	1:D:351:ILE:HD11	2.01	0.42
1:J:238:ASP:OD2	1:J:240:THR:CB	2.68	0.42
1:J:451:SER:O	1:J:452:SER:CB	2.67	0.42
1:D:274:LYS:HG3	1:D:275:GLU:OE2	2.20	0.42
2:E:972:ILE:HG12	2:E:995:VAL:HG22	1.99	0.42
2:E:1037:LEU:N	2:E:1038:PRO:CD	2.82	0.42
1:G:252:GLN:HG3	1:G:335:MSE:SE	2.69	0.42
1:J:440:MSE:HE2	1:J:440:MSE:HB2	1.98	0.42
1:A:168:LYS:O	1:A:178:ARG:HD3	2.19	0.42
1:A:188:SER:HB3	1:A:190:ASP:OD1	2.20	0.42
1:D:135:LYS:HD2	1:D:191:GLY:HA3	2.01	0.42
1:D:316:CYS:SG	1:D:324:LEU:HG	2.59	0.42
1:G:247:ARG:NH1	1:G:338:ASP:OD2	2.50	0.42
1:J:148:ASP:HB3	1:J:150:THR:CB	2.43	0.42
1:J:358:ARG:NH2	1:J:380:ILE:HD12	2.33	0.42
2:K:1065:THR:HG22	2:K:1067:LYS:CG	2.49	0.42
1:D:14:GLN:O	1:D:15:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:GLY:O	1:D:408:LEU:C	2.62	0.42
1:J:135:LYS:HD2	1:J:191:GLY:HA3	2.02	0.42
1:A:120:GLU:H	1:A:120:GLU:HG3	1.47	0.42
1:D:276:TYR:CD2	4:D:6119:PGE:H5	2.53	0.42
2:E:1079:ARG:O	2:E:1083:ARG:HG2	2.20	0.42
1:G:407:GLY:O	1:G:408:LEU:C	2.63	0.42
1:A:358:ARG:NH2	1:A:380:ILE:HD12	2.34	0.42
2:B:983:SER:C	2:B:985:LEU:N	2.76	0.42
1:D:199:THR:O	1:D:199:THR:CG2	2.68	0.42
1:G:386:PHE:HB2	1:G:389:TRP:CE2	2.54	0.42
1:J:50:THR:HG22	1:J:51:ASP:OD1	2.20	0.42
1:A:290:PHE:HA	1:A:291:PRO:HD3	1.86	0.42
1:D:325:ILE:HG13	1:D:325:ILE:O	2.18	0.42
2:E:1010:ASP:HB3	2:E:1046:GLY:HA2	2.02	0.42
3:F:1450:GLY:O	3:F:1454:LYS:HG3	2.20	0.42
1:A:119:GLU:O	1:A:120:GLU:C	2.63	0.42
1:D:101:GLU:O	1:D:102:ASP:C	2.63	0.42
1:D:242:ASP:OD1	1:D:242:ASP:C	2.63	0.42
2:E:972:ILE:CG2	2:E:973:SER:N	2.83	0.42
2:E:1015:PRO:O	2:E:1017:THR:N	2.52	0.42
1:G:28:SER:HA	1:G:34:ARG:O	2.19	0.42
1:G:82:LEU:HD12	1:G:82:LEU:H	1.84	0.42
1:G:146:LYS:C	1:G:148:ASP:N	2.76	0.42
1:J:28:SER:HA	1:J:34:ARG:O	2.19	0.42
1:J:343:VAL:CG1	2:K:1066:ARG:CZ	2.95	0.42
1:A:213:PRO:O	1:A:277:ARG:HD3	2.19	0.42
1:A:239:SER:HA	1:A:246:LYS:NZ	2.34	0.42
1:A:288:ASN:O	1:A:349:VAL:HA	2.20	0.42
1:D:10:LEU:HG	1:D:11:PRO:HD2	2.02	0.42
1:D:43:ILE:O	1:D:56:SER:HA	2.19	0.42
1:D:119:GLU:O	1:D:120:GLU:C	2.63	0.42
1:G:358:ARG:NH2	1:G:380:ILE:HD12	2.34	0.42
2:H:972:ILE:HG12	2:H:995:VAL:HG22	2.02	0.42
1:J:101:GLU:O	1:J:102:ASP:C	2.63	0.42
1:J:146:LYS:C	1:J:148:ASP:N	2.76	0.42
2:K:972:ILE:CG2	2:K:973:SER:N	2.82	0.42
1:A:50:THR:HG22	1:A:51:ASP:OD1	2.19	0.41
1:D:380:ILE:HG21	1:D:382:GLN:HG3	2.01	0.41
1:G:119:GLU:O	1:G:120:GLU:C	2.63	0.41
1:G:332:GLU:HG2	3:I:1443:MSE:HE3	2.02	0.41
1:G:451:SER:O	1:G:452:SER:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:LYS:O	1:J:178:ARG:HD3	2.20	0.41
1:A:15:ALA:HB2	1:A:39:GLN:OE1	2.19	0.41
2:B:1061:VAL:CG1	2:B:1066:ARG:HA	2.51	0.41
2:B:1065:THR:HG22	2:B:1067:LYS:CG	2.49	0.41
2:B:1079:ARG:O	2:B:1083:ARG:HG2	2.20	0.41
3:C:1437:VAL:O	3:C:1441:LEU:HG	2.21	0.41
1:G:50:THR:HG22	1:G:51:ASP:OD1	2.21	0.41
2:H:1054:THR:HG23	2:H:1103:VAL:HG22	2.01	0.41
1:J:33:THR:HG22	1:J:34:ARG:HG3	2.01	0.41
1:A:101:GLU:O	1:A:102:ASP:C	2.64	0.41
1:G:210:PRO:HB2	1:G:212:LEU:HG	2.02	0.41
1:G:380:ILE:HG21	1:G:382:GLN:HG3	2.02	0.41
1:A:252:GLN:HG3	1:A:335:MSE:SE	2.70	0.41
2:B:966:MSE:HE2	2:B:1020:GLY:CA	2.50	0.41
1:D:451:SER:O	1:D:452:SER:CB	2.68	0.41
2:E:1006:LEU:HD21	2:E:1052:ARG:NH1	2.35	0.41
2:H:966:MSE:HE2	2:H:1020:GLY:CA	2.51	0.41
1:J:213:PRO:O	1:J:277:ARG:HD3	2.20	0.41
2:K:966:MSE:HE2	2:K:1020:GLY:CA	2.50	0.41
1:A:302:ILE:HA	1:A:316:CYS:O	2.21	0.41
1:D:146:LYS:C	1:D:148:ASP:N	2.77	0.41
1:D:229:LYS:HE3	1:D:332:GLU:CD	2.45	0.41
1:D:381:ILE:O	1:D:417:ILE:HB	2.20	0.41
1:G:30:GLN:HB2	1:G:33:THR:HG22	2.02	0.41
1:G:101:GLU:O	1:G:102:ASP:C	2.62	0.41
1:G:189:LYS:NZ	1:G:304:THR:HG22	2.36	0.41
1:G:210:PRO:CD	1:G:335:MSE:HE3	2.50	0.41
1:G:440:MSE:HE2	1:G:440:MSE:HB2	2.00	0.41
2:H:1067:LYS:HA	2:H:1068:PRO:HD3	1.90	0.41
1:J:7:LEU:HB2	1:J:431:TRP:CE3	2.55	0.41
1:A:146:LYS:C	1:A:148:ASP:N	2.76	0.41
1:D:137:TYR:CD2	1:D:138:ARG:HG3	2.56	0.41
2:E:1061:VAL:CG1	2:E:1066:ARG:HA	2.51	0.41
1:G:43:ILE:O	1:G:56:SER:HA	2.20	0.41
1:G:212:LEU:O	1:G:277:ARG:HD2	2.21	0.41
2:H:1030:THR:CG2	2:H:1031:CYS:N	2.83	0.41
1:J:252:GLN:HG3	1:J:335:MSE:SE	2.71	0.41
1:D:252:GLN:HG3	1:D:335:MSE:SE	2.71	0.41
2:E:1060:PRO:HG3	2:E:1080:HIS:CD2	2.56	0.41
2:E:1084:LEU:C	2:E:1086:LYS:N	2.78	0.41
2:E:1088:PRO:C	2:E:1090:SER:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:HIS:HA	1:G:134:PRO:HD3	1.93	0.41
1:J:93:VAL:HA	1:J:94:PRO:HD3	1.90	0.41
1:A:7:LEU:HG	1:A:9:ALA:HB3	2.02	0.41
2:B:972:ILE:CG2	2:B:973:SER:N	2.83	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CE2	2.55	0.41
2:E:1030:THR:CG2	2:E:1031:CYS:N	2.84	0.41
1:G:179:VAL:HG21	1:G:281:VAL:HG11	2.01	0.41
1:G:321:ASP:OD2	1:G:353:ARG:NH2	2.54	0.41
1:G:402:LEU:HD21	3:I:1448:GLN:CB	2.50	0.41
2:H:983:SER:C	2:H:985:LEU:N	2.78	0.41
2:H:1015:PRO:O	2:H:1017:THR:N	2.54	0.41
1:J:288:ASN:O	1:J:349:VAL:HA	2.21	0.41
1:J:289:PRO:HD2	1:J:350:LEU:HB3	2.02	0.41
1:J:386:PHE:HB2	1:J:389:TRP:CZ2	2.55	0.41
1:A:291:PRO:HB2	1:A:294:LEU:HD12	2.03	0.41
1:A:451:SER:O	1:A:452:SER:CB	2.68	0.41
1:D:444:THR:CG2	1:D:445:LEU:N	2.74	0.41
2:E:983:SER:C	2:E:985:LEU:N	2.77	0.41
1:G:238:ASP:CG	1:G:239:SER:N	2.78	0.41
1:J:26:ILE:HB	1:J:440:MSE:HE3	2.03	0.41
1:J:133:HIS:HA	1:J:134:PRO:HD3	1.92	0.41
1:J:332:GLU:HG2	3:L:1443:MSE:HE3	2.01	0.41
2:K:1030:THR:CG2	2:K:1031:CYS:N	2.82	0.41
1:D:168:LYS:O	1:D:178:ARG:HD3	2.21	0.41
1:D:240:THR:OG1	1:G:9:ALA:HB2	2.21	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CZ2	2.56	0.41
1:G:290:PHE:HA	1:G:291:PRO:HD3	1.86	0.41
1:G:291:PRO:HB2	1:G:294:LEU:HD12	2.02	0.41
1:J:137:TYR:CD2	1:J:138:ARG:HG3	2.56	0.41
1:J:274:LYS:HG3	1:J:275:GLU:OE2	2.20	0.41
2:K:1054:THR:HG23	2:K:1103:VAL:HG22	2.03	0.41
1:A:372:LYS:HE2	1:A:385:ASN:HD21	1.84	0.40
1:D:251:LYS:HB3	4:D:6119:PGE:H62	2.03	0.40
1:G:135:LYS:HD2	1:G:191:GLY:HA3	2.03	0.40
1:G:316:CYS:SG	1:G:324:LEU:HG	2.61	0.40
1:J:210:PRO:HB2	1:J:212:LEU:HG	2.03	0.40
1:A:7:LEU:C	1:A:9:ALA:H	2.29	0.40
1:A:228:ASN:ND2	3:C:1435:LYS:HB2	2.36	0.40
2:B:1047:ILE:O	2:B:1047:ILE:HG22	2.20	0.40
2:K:983:SER:C	2:K:985:LEU:N	2.77	0.40
1:G:386:PHE:HB2	1:G:389:TRP:CZ2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:966:MSE:HG3	2:H:1020:GLY:CA	2.50	0.40
1:J:242:ASP:OD1	1:J:242:ASP:C	2.64	0.40
1:J:302:ILE:HA	1:J:316:CYS:O	2.21	0.40
1:J:321:ASP:OD2	1:J:353:ARG:NH2	2.54	0.40
1:D:179:VAL:HG21	1:D:281:VAL:HG11	2.04	0.40
2:E:1047:ILE:O	2:E:1047:ILE:HG22	2.20	0.40
1:J:290:PHE:HA	1:J:291:PRO:HD3	1.85	0.40
2:K:988:ARG:HA	2:K:1010:ASP:HA	2.02	0.40
2:H:1061:VAL:CG1	2:H:1066:ARG:HA	2.52	0.40
1:J:343:VAL:HG12	1:J:344:TYR:N	2.36	0.40
2:K:1087:ASN:N	2:K:1088:PRO:HD3	2.36	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	432/452 (96%)	396 (92%)	32 (7%)	4 (1%)	14	30
1	D	431/452 (95%)	397 (92%)	29 (7%)	5 (1%)	10	23
1	G	432/452 (96%)	396 (92%)	32 (7%)	4 (1%)	14	30
1	J	433/452 (96%)	399 (92%)	29 (7%)	5 (1%)	10	23
2	B	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	3	4
2	E	144/148 (97%)	117 (81%)	20 (14%)	7 (5%)	1	2
2	H	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	4	6
2	K	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	3	4
3	C	24/36 (67%)	21 (88%)	2 (8%)	1 (4%)	2	3
3	F	24/36 (67%)	21 (88%)	3 (12%)	0	100	100
3	I	26/36 (72%)	25 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	22/36 (61%)	21 (96%)	1 (4%)	0	100	100
All	All	2400/2544 (94%)	2154 (90%)	206 (9%)	40 (2%)	7	15

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	TYR
2	B	1036	ASN
3	C	1435	LYS
1	D	344	TYR
1	G	344	TYR
1	J	344	TYR
2	B	1016	LEU
2	E	1016	LEU
1	G	339	VAL
2	H	1016	LEU
1	J	339	VAL
2	K	1016	LEU
1	A	339	VAL
2	B	975	SER
1	D	339	VAL
2	E	975	SER
2	E	1040	ARG
2	H	975	SER
2	K	975	SER
2	K	1036	ASN
1	A	200	THR
1	D	10	LEU
2	H	1036	ASN
2	B	1087	ASN
1	D	200	THR
1	J	200	THR
2	E	1036	ASN
2	E	1038	PRO
2	E	1088	PRO
1	G	200	THR
2	K	1046	GLY
2	B	1046	GLY
2	E	1046	GLY
2	H	1046	GLY
1	A	423	ILE
1	G	423	ILE

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Mol	Chain	Res	Type
1	J	12	ILE
1	J	423	ILE
2	K	1087	ASN
1	D	423	ILE

5.3.2 Protein sidechains ⓘ

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	411/415 (99%)	392 (95%)	19 (5%)	24	49
1	D	410/415 (99%)	390 (95%)	20 (5%)	22	47
1	G	411/415 (99%)	392 (95%)	19 (5%)	24	49
1	J	412/415 (99%)	393 (95%)	19 (5%)	24	49
2	B	132/133 (99%)	129 (98%)	3 (2%)	44	71
2	E	132/133 (99%)	129 (98%)	3 (2%)	44	71
2	H	132/133 (99%)	129 (98%)	3 (2%)	44	71
2	K	132/133 (99%)	129 (98%)	3 (2%)	44	71
3	C	22/28 (79%)	22 (100%)	0	100	100
3	F	22/28 (79%)	21 (96%)	1 (4%)	24	50
3	I	24/28 (86%)	22 (92%)	2 (8%)	10	23
3	L	21/28 (75%)	21 (100%)	0	100	100
All	All	2261/2304 (98%)	2169 (96%)	92 (4%)	27	54

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	29	SER
1	A	33	THR
1	A	71	VAL
1	A	100	VAL
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	102	ASP
1	A	120	GLU
1	A	148	ASP
1	A	176	ASP
1	A	185	LEU
1	A	210	PRO
1	A	217	LEU
1	A	281	VAL
1	A	286	THR
1	A	304	THR
1	A	307	ILE
1	A	324	LEU
1	A	365	THR
2	B	968	GLU
2	B	1049	VAL
2	B	1098	ASP
1	D	8	SER
1	D	29	SER
1	D	33	THR
1	D	50	THR
1	D	71	VAL
1	D	100	VAL
1	D	101	GLU
1	D	102	ASP
1	D	120	GLU
1	D	148	ASP
1	D	176	ASP
1	D	185	LEU
1	D	210	PRO
1	D	217	LEU
1	D	281	VAL
1	D	286	THR
1	D	304	THR
1	D	307	ILE
1	D	324	LEU
1	D	365	THR
2	E	968	GLU
2	E	1049	VAL
2	E	1098	ASP
3	F	1434	PHE
1	G	29	SER
1	G	33	THR

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Mol	Chain	Res	Type
1	G	71	VAL
1	G	100	VAL
1	G	101	GLU
1	G	102	ASP
1	G	120	GLU
1	G	148	ASP
1	G	176	ASP
1	G	185	LEU
1	G	210	PRO
1	G	217	LEU
1	G	281	VAL
1	G	286	THR
1	G	304	THR
1	G	307	ILE
1	G	324	LEU
1	G	365	THR
1	G	402	LEU
2	H	968	GLU
2	H	1049	VAL
2	H	1098	ASP
3	I	1430	ASP
3	I	1456	LEU
1	J	29	SER
1	J	33	THR
1	J	71	VAL
1	J	100	VAL
1	J	101	GLU
1	J	102	ASP
1	J	120	GLU
1	J	148	ASP
1	J	176	ASP
1	J	185	LEU
1	J	210	PRO
1	J	217	LEU
1	J	281	VAL
1	J	286	THR
1	J	304	THR
1	J	307	ILE
1	J	324	LEU
1	J	365	THR
1	J	442	ASN
2	K	968	GLU

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Mol	Chain	Res	Type
2	K	1049	VAL
2	K	1098	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	106	GLN
1	A	180	ASN
1	A	262	ASN
1	A	383	GLN
1	A	434	GLN
1	A	449	ASN
2	B	967	ASN
2	B	969	ASN
2	B	1074	HIS
2	B	1087	ASN
1	D	31	ASN
1	D	106	GLN
1	D	180	ASN
1	D	228	ASN
1	D	262	ASN
1	D	383	GLN
1	D	434	GLN
1	D	449	ASN
2	E	967	ASN
2	E	969	ASN
2	E	1074	HIS
2	E	1075	GLN
3	F	1448	GLN
3	F	1457	ASN
1	G	31	ASN
1	G	62	HIS
1	G	106	GLN
1	G	180	ASN
1	G	262	ASN
1	G	383	GLN
1	G	434	GLN
1	G	449	ASN
2	H	967	ASN
2	H	969	ASN
2	H	1039	ASN

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Mol	Chain	Res	Type
2	H	1074	HIS
2	H	1075	GLN
2	H	1087	ASN
2	H	1108	HIS
3	I	1448	GLN
1	J	106	GLN
1	J	180	ASN
1	J	262	ASN
1	J	312	ASN
1	J	434	GLN
1	J	449	ASN
2	K	967	ASN
2	K	969	ASN
2	K	1074	HIS
2	K	1087	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	D	6119	-	9,9,9	0.93	1 (11%)	8,8,8	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	D	6119	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6119	PGE	C5-C6	2.25	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6119	PGE	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6119	PGE	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

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, 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	431/452 (95%)	0.71	32 (7%)	20 16	44, 65, 96, 118	0
1	D	430/452 (95%)	0.65	30 (6%)	22 18	41, 65, 98, 118	0
1	G	431/452 (95%)	0.66	21 (4%)	35 29	43, 65, 97, 117	0
1	J	432/452 (95%)	0.66	26 (6%)	27 22	41, 64, 99, 117	0
2	B	145/148 (97%)	1.28	26 (17%)	3 3	53, 90, 116, 129	0
2	E	145/148 (97%)	1.44	31 (21%)	2 2	52, 90, 116, 129	0
2	H	145/148 (97%)	1.74	49 (33%)	1 1	58, 94, 119, 144	0
2	K	145/148 (97%)	1.16	21 (14%)	6 4	56, 92, 117, 137	0
3	C	24/36 (66%)	0.88	2 (8%)	17 13	59, 69, 91, 108	0
3	F	24/36 (66%)	0.90	3 (12%)	8 6	58, 69, 89, 109	0
3	I	26/36 (72%)	0.86	2 (7%)	19 15	57, 71, 118, 123	0
3	L	23/36 (63%)	0.74	1 (4%)	40 34	62, 70, 89, 96	0
All	All	2401/2544 (94%)	0.85	244 (10%)	12 9	41, 70, 106, 144	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1076	LEU	5.1
2	H	1019	LEU	5.1
2	H	1038	PRO	4.8
2	B	1076	LEU	4.7
1	G	7	LEU	4.7
1	D	7	LEU	4.6
1	A	175	LEU	4.4
1	A	7	LEU	4.3
1	G	175	LEU	4.2
2	B	1047	ILE	4.2
2	E	1035	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	984	LEU	4.0
2	H	1037	LEU	4.0
2	H	1044	GLY	3.9
1	J	23	PRO	3.9
1	G	176	ASP	3.9
1	A	424	PRO	3.8
1	A	423	ILE	3.8
2	K	1047	ILE	3.8
2	E	1097	ALA	3.7
3	C	1434	PHE	3.7
1	D	318	SER	3.7
2	B	1098	ASP	3.7
1	D	175	LEU	3.7
2	H	1034	TYR	3.7
2	K	1038	PRO	3.7
2	K	984	LEU	3.6
2	H	982	TYR	3.6
2	H	1032	ILE	3.6
2	E	1021	GLY	3.6
2	K	1032	ILE	3.6
2	E	1089	ASN	3.5
2	E	1098	ASP	3.5
2	H	987	LEU	3.5
1	D	423	ILE	3.5
2	E	1047	ILE	3.5
2	H	1035	ALA	3.4
1	J	175	LEU	3.4
2	H	974	PRO	3.4
2	E	1022	VAL	3.4
1	G	423	ILE	3.3
1	G	123	PRO	3.3
2	B	1072	PRO	3.3
1	J	423	ILE	3.3
1	G	173	PHE	3.3
2	B	972	ILE	3.3
1	A	103	VAL	3.3
2	B	1037	LEU	3.2
2	H	1016	LEU	3.2
1	A	123	PRO	3.2
2	H	985	LEU	3.2
1	J	176	ASP	3.2
2	K	1019	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	L	1434	PHE	3.2
2	E	1072	PRO	3.1
2	H	1017	THR	3.1
1	J	452	SER	3.1
1	D	156	ILE	3.1
1	D	380	ILE	3.1
2	H	976	LEU	3.0
2	H	979	LEU	3.0
2	H	977	ASP	3.0
2	B	1097	ALA	3.0
2	K	1049	VAL	3.0
2	H	1042	LYS	3.0
3	F	1434	PHE	3.0
2	H	992	HIS	3.0
2	K	967	ASN	3.0
2	K	1034	TYR	3.0
2	E	1037	LEU	2.9
2	H	970	TYR	2.9
2	K	982	TYR	2.9
2	H	1076	LEU	2.9
2	H	1015	PRO	2.9
1	G	400	SER	2.9
1	D	40	ASP	2.9
2	H	1014	ILE	2.9
1	A	176	ASP	2.9
2	E	970	TYR	2.9
1	A	23	PRO	2.9
2	K	1035	ALA	2.9
1	J	109	PHE	2.9
2	H	1111	GLU	2.8
2	E	1046	GLY	2.8
1	D	100	VAL	2.8
2	E	1010	ASP	2.8
2	B	1035	ALA	2.8
1	A	431	TRP	2.8
2	B	1057	ASN	2.8
1	D	401	ASP	2.8
2	H	1049	VAL	2.8
2	H	972	ILE	2.8
1	D	421	GLU	2.7
1	J	123	PRO	2.7
2	B	1024	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	408	LEU	2.7
2	E	1019	LEU	2.7
3	I	1434	PHE	2.7
1	A	452	SER	2.7
1	D	161	GLU	2.7
2	K	985	LEU	2.7
1	J	377	SER	2.7
1	D	15	ALA	2.7
2	H	1081	ILE	2.6
1	A	411	GLU	2.6
2	H	1023	ILE	2.6
2	H	1030	THR	2.6
2	H	971	TYR	2.6
1	J	100	VAL	2.6
2	B	1041	PRO	2.6
2	H	1018	SER	2.6
2	K	1037	LEU	2.6
2	B	1074	HIS	2.6
2	K	968	GLU	2.6
2	E	1020	GLY	2.6
2	H	990	VAL	2.6
2	H	991	PRO	2.6
1	D	120	GLU	2.5
2	H	1101	THR	2.5
1	J	431	TRP	2.5
2	E	1029	LYS	2.5
2	K	1111	GLU	2.5
2	B	985	LEU	2.5
2	K	1079	ARG	2.5
1	D	23	PRO	2.5
1	G	23	PRO	2.5
2	B	1026	PHE	2.5
1	J	420	ILE	2.5
2	E	1032	ILE	2.5
2	B	1038	PRO	2.5
2	E	1034	TYR	2.5
2	H	1022	VAL	2.5
1	G	402	LEU	2.4
2	H	1047	ILE	2.4
1	J	172	SER	2.4
1	J	318	SER	2.4
2	E	1090	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	1000	TYR	2.4
2	E	1025	THR	2.4
1	J	171	ASN	2.4
2	E	1024	ILE	2.4
1	D	177	ALA	2.4
1	A	450	ILE	2.4
2	E	984	LEU	2.4
2	E	1033	ILE	2.4
2	H	1024	ILE	2.4
2	K	1016	LEU	2.4
2	K	1030	THR	2.4
1	G	172	SER	2.4
2	H	1029	LYS	2.4
2	H	984	LEU	2.4
1	J	170	ASN	2.4
2	E	1075	GLN	2.4
1	J	405	LEU	2.3
1	G	318	SER	2.3
1	J	434	GLN	2.3
2	H	986	GLN	2.3
2	E	1005	PHE	2.3
2	K	1033	ILE	2.3
1	J	421	GLU	2.3
2	E	1085	LYS	2.3
1	A	401	ASP	2.3
1	G	174	GLY	2.3
1	J	6	ARG	2.3
2	E	1009	VAL	2.3
2	H	994	VAL	2.3
1	J	53	LEU	2.3
1	A	180	ASN	2.3
2	E	1038	PRO	2.3
2	K	1076	LEU	2.3
3	F	1439	VAL	2.3
2	H	1033	ILE	2.2
1	D	240	THR	2.2
1	A	174	GLY	2.2
2	B	1071	ASP	2.2
2	B	1100	GLY	2.2
1	A	53	LEU	2.2
1	A	177	ALA	2.2
1	G	436	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	234	TYR	2.2
1	A	433	ASP	2.2
1	J	98	SER	2.2
2	B	1016	LEU	2.2
2	H	973	SER	2.2
1	G	100	VAL	2.2
1	A	420	ILE	2.2
1	G	450	ILE	2.2
2	K	1026	PHE	2.2
1	D	53	LEU	2.2
2	B	1046	GLY	2.2
2	H	1011	LEU	2.2
1	G	401	ASP	2.2
1	A	318	SER	2.2
1	D	452	SER	2.2
1	G	391	SER	2.2
2	B	1077	VAL	2.2
1	D	171	ASN	2.1
2	B	1085	LYS	2.1
2	H	1059	TYR	2.1
2	E	985	LEU	2.1
1	J	179	VAL	2.1
1	J	236	SER	2.1
1	J	384	VAL	2.1
1	A	173	PHE	2.1
1	D	173	PHE	2.1
1	G	443	LYS	2.1
2	B	1075	GLN	2.1
1	A	414	LEU	2.1
3	F	1457	ASN	2.1
1	D	234	TYR	2.1
3	I	1456	LEU	2.1
2	H	1077	VAL	2.1
1	A	410	PHE	2.1
1	A	406	ALA	2.1
1	D	299	ALA	2.1
1	G	399	GLU	2.1
1	D	11	PRO	2.1
1	D	228	ASN	2.1
3	C	1433	GLY	2.1
1	D	201	GLU	2.1
1	D	411	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	443	LYS	2.1
1	A	240	THR	2.1
2	K	1025	THR	2.1
2	H	1041	PRO	2.1
1	A	171	ASN	2.1
1	G	343	VAL	2.1
1	D	149	ASP	2.0
1	D	176	ASP	2.0
2	E	1043	ARG	2.0
1	G	452	SER	2.0
1	A	398	ASN	2.0
1	A	442	ASN	2.0
1	D	420	ILE	2.0
2	B	1032	ILE	2.0
2	B	1034	TYR	2.0
1	A	149	ASP	2.0
1	D	451	SER	2.0
2	E	1108	HIS	2.0
1	A	449	ASN	2.0
2	B	1033	ILE	2.0
2	H	1001	GLY	2.0
1	A	100	VAL	2.0
2	H	1009	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGE	D	6119	10/10	0.80	0.18	70,72,77,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.