



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:22 AM GMT

PDB ID : 3PBP
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 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/ValidationPDFNotes.html>

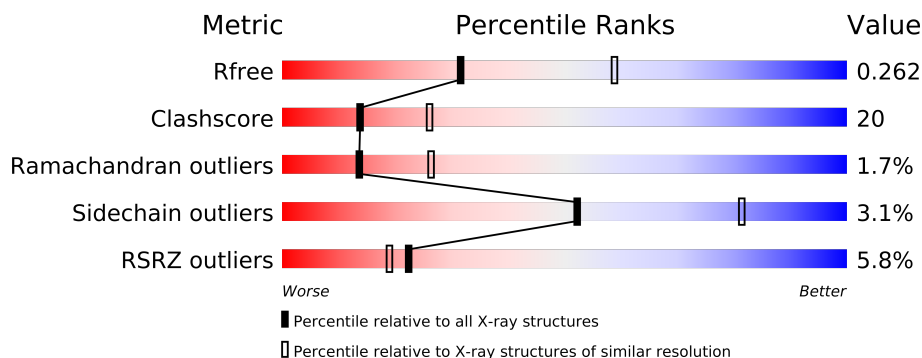
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	452	
1	D	452	
1	G	452	
1	J	452	
2	B	148	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	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 hydrogen and 0 are deuterium.

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			

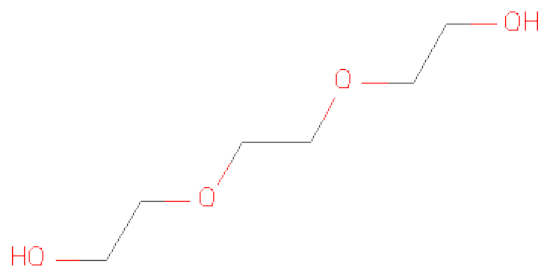
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: PGE) (formula: C₆H₁₄O₄).



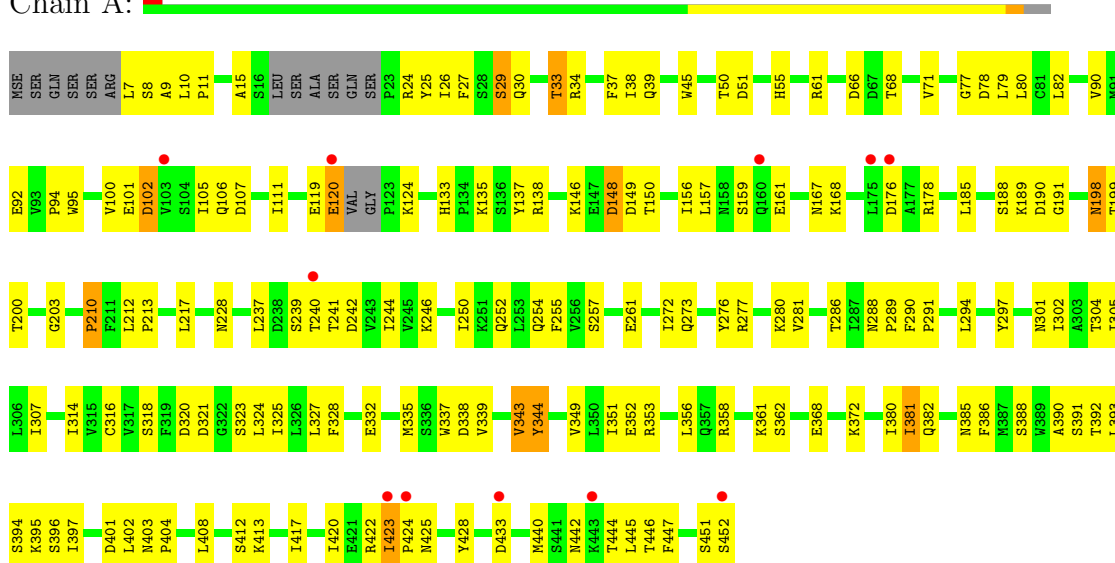
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	6	4		

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

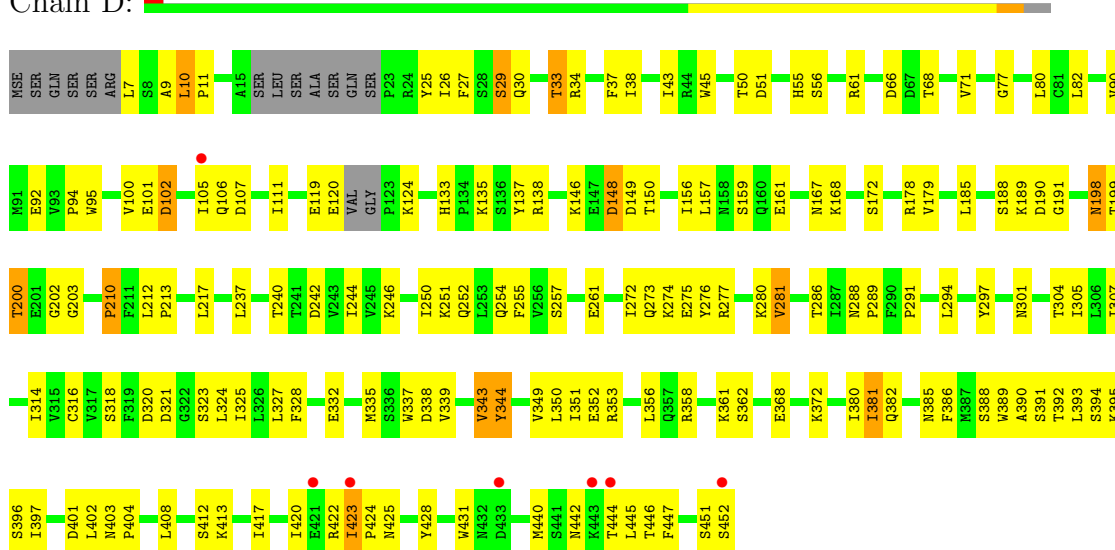
• Molecule 1: Nucleoporin NUP82

Chain A:



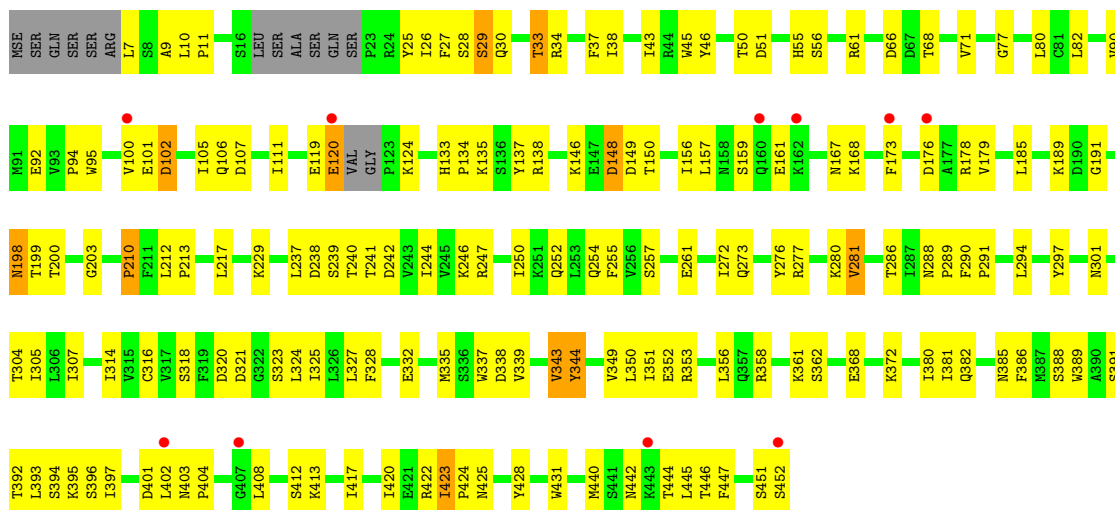
• Molecule 1: Nucleoporin NUP82

Chain D:



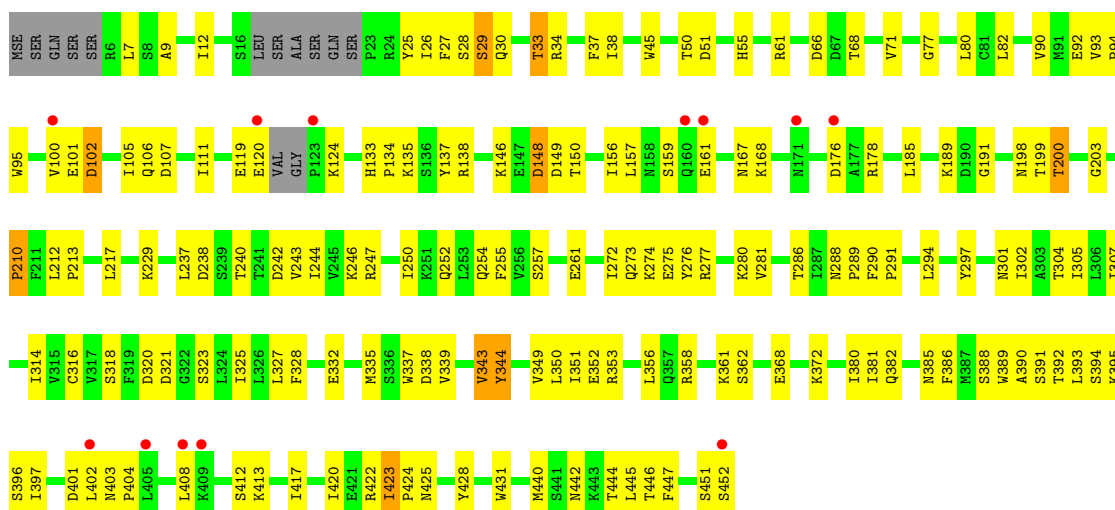
• Molecule 1: Nucleoporin NUP82

Chain G:



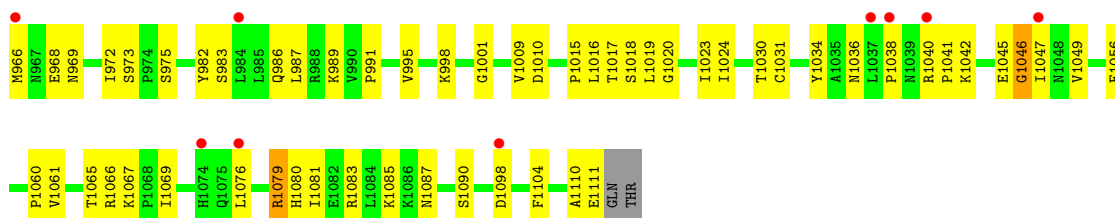
• Molecule 1: Nucleoporin NUP82

Chain J:



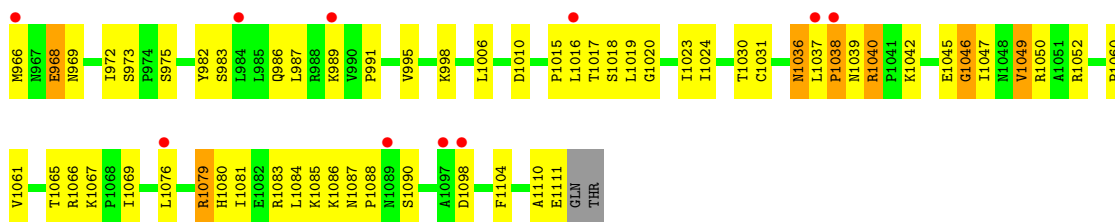
• Molecule 2: Nucleoporin NUP116/NSP116

Chain B:



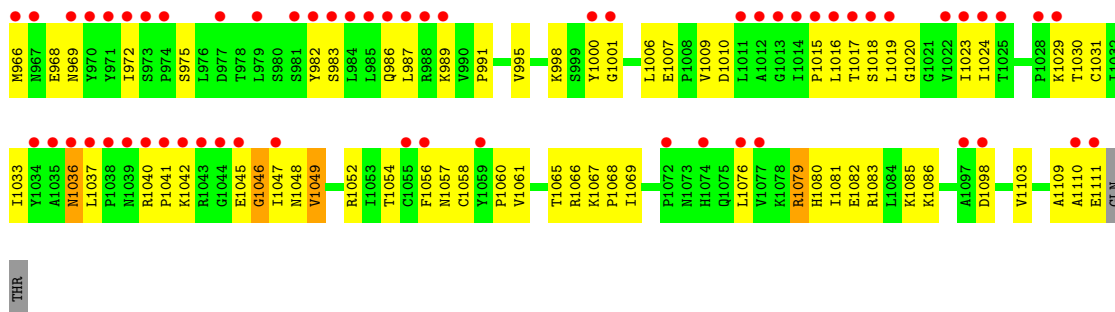
• Molecule 2: Nucleoporin NUP116/NSP116

Chain E:



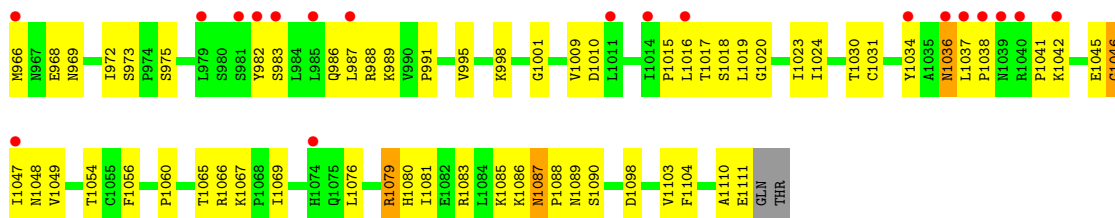
• Molecule 2: Nucleoporin NUP116/NSP116

Chain H:



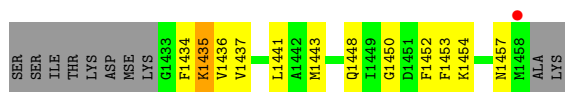
• Molecule 2: Nucleoporin NUP116/NSP116

Chain K:



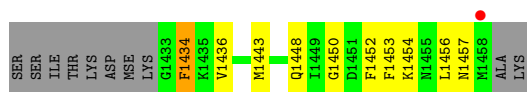
• Molecule 3: Nucleoporin NUP159

Chain C:



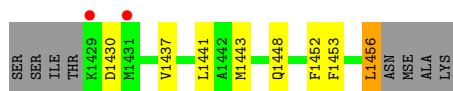
• Molecule 3: Nucleoporin NUP159

Chain F:



• Molecule 3: Nucleoporin NUP159

Chain I:



● Molecule 3: Nucleoporin NUP159

Chain L:

SER	SER	ILE	THR	LYS	ASP	MSF	LYS	GLY	F1434	M1443	Q1448	F1452	F1453	L1456	N1457	MSF	ALA	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----

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 47.11 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 93.4 (47.11-2.81)	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 0.237 , 0.262	Depositor DCC
R_{free} test set	6672 reflections (10.89%)	DCC
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 , 39.4	EDS
Estimated twinning fraction	0.013 for -h,-k,h+k+l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70324 reflections	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.

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	0.43	0/3603	0.68	2/4877 (0.0%)
1	D	0.42	0/3597	0.68	2/4869 (0.0%)
1	G	0.42	0/3603	0.68	1/4877 (0.0%)
1	J	0.43	0/3614	0.68	1/4891 (0.0%)
2	B	0.35	0/1193	0.64	0/1617
2	E	0.35	0/1193	0.62	0/1617
2	H	0.41	0/1193	0.63	0/1617
2	K	0.37	0/1193	0.63	0/1617
3	C	0.53	0/204	0.61	0/266
3	F	0.48	0/204	0.56	0/266
3	I	0.44	0/222	0.64	0/288
3	L	0.49	0/193	0.52	0/254
All	All	0.41	0/20012	0.66	6/27056 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	343	VAL	N-CA-C	-5.42	96.38	111.00
1	G	343	VAL	N-CA-C	-5.15	97.09	111.00
1	D	343	VAL	N-CA-C	-5.10	97.23	111.00
1	A	343	VAL	N-CA-C	-5.05	97.36	111.00
1	A	381	ILE	N-CA-C	-5.04	97.38	111.00
1	D	381	ILE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	3507	141	0
1	D	3533	0	3502	146	0
1	G	3539	0	3507	154	0
1	J	3550	0	3520	157	0
2	B	1165	0	1183	39	0
2	E	1165	0	1183	46	0
2	H	1165	0	1183	54	0
2	K	1165	0	1183	46	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	5	0
All	All	19653	0	19646	784	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (784) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:G:210:PRO:CG	1:G:335:MSE:HE3	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:983:SER:HB2	2:H:986:GLN:HG2	1.64	0.80
2:E:983:SER:HB2	2:E:986:GLN:HG2	1.64	0.80
1:G:90:VAL:HG11	1:G:156:ILE:HD13	1.62	0.80
1:D:148:ASP:HB3	1:D:150:THR:HB	1.64	0.79
1:A:92:GLU:HB2	1:A:111:ILE:HD11	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
1:D:381:ILE:HD11	1:D:424:PRO:HG3	1.66	0.77
2:E:1038:PRO:C	2:E:1040:ARG:H	1.85	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
3:I:1441:LEU:HD11	1:J:243:VAL:HG13	1.68	0.76
1:A:280:LYS:HD2	1:A:338:ASP:O	1.85	0.76
1:D:358:ARG:CZ	1:D:380:ILE:HD12	2.17	0.75
1:J:358:ARG:CZ	1:J:380:ILE:HD12	2.16	0.75
1:J:148:ASP:HB3	1:J:150:THR:HB	1.67	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
1:G:255:PHE:CD2	1:G:335:MSE:HE1	2.22	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:J:361:LYS:HE2	1:J:423:ILE:HD11	1.69	0.74
1:G:280:LYS:HD2	1:G:338:ASP:O	1.87	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:J:119:GLU:O	1:J:124:LYS:HE2	1.88	0.73
1:D:27:PHE:HZ	1:D:71:VAL:HG23	1.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:J:335:MSE:HE2	1:J:337:TRP:CZ2	2.25	0.72
1:J:66:ASP:OD1	1:J:68:THR:HB	1.89	0.72
1:A:392:THR:HG21	1:A:408:LEU:HD11	1.72	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:J:37:PHE:HE1	1:J:440:MSE:HE1	1.54	0.72
1:G:189:LYS:HG2	1:G:304:THR:CG2	2.19	0.72
1:G:66:ASP:OD1	1:G:68:THR:HB	1.90	0.72
1:D:444:THR:HG22	1:D:445:LEU:N	2.04	0.72
1:D:335:MSE:HE2	1:D:337:TRP:CZ2	2.23	0.72
1:A:119:GLU:O	1:A:124:LYS:HE2	1.89	0.72
1:J:444:THR:HG22	1:J:445:LEU:N	2.05	0.72
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
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:444:THR:HG22	1:G:445:LEU:N	2.05	0.71
1:G:361:LYS:HE2	1:G:423:ILE:HD11	1.72	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:G:7:LEU:HB2	1:G:431:TRP:CZ3	2.27	0.69
1:A:189:LYS:HG2	1:A:304:THR:CG2	2.22	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:440:MSE:HE2	1:D:445:LEU:HD13	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:361:LYS:HE2	1:D:423:ILE:HD11	1.74	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:J:422:ARG:HG3	1:J:442:ASN:HD21	1.58	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
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
1:J:335:MSE:HE2	1:J:337:TRP:CH2	2.31	0.65
1:D:422:ARG:HG3	1:D:442:ASN:HD21	1.61	0.65
1:A:422:ARG:HG3	1:A:442:ASN:HD21	1.61	0.65
2:H:1010:ASP:HB3	2:H:1046:GLY:CA	2.21	0.65
1:J:440:MSE:HE2	1:J:445:LEU:HD13	1.76	0.65
1:J:189:LYS:HG2	1:J:304:THR:CG2	2.26	0.65
1:G:440:MSE:HE2	1:G:445:LEU:HD13	1.78	0.65
1:D:343:VAL:HG11	2:E:1066:ARG:CZ	2.26	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:92:GLU:HB2	1:J:111:ILE:CD1	2.26	0.64
1:J:34:ARG:HB3	1:J:95:TRP:CH2	2.31	0.64
1:G:255:PHE:CE2	1:G:335:MSE:HE1	2.32	0.64
1:G:34:ARG:HB3	1:G:95:TRP:CH2	2.32	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
1:A:301:ASN:H	1:A:318:SER:HB2	1.63	0.64
1:G:30:GLN:O	1:G:33:THR:HB	1.97	0.64
2:B:1090:SER:HB2	2:B:1104:PHE:CD2	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:92:GLU:HB2	1:D:111:ILE:CD1	2.26	0.63
1:D:25:TYR:CD2	1:D:71:VAL:HG22	2.33	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
1:D:26:ILE:HB	1:D:440:MSE:HE3	1.80	0.62
2:B:1015:PRO:HG2	2:B:1018:SER:OG	1.99	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
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:J:444:THR:CG2	1:J:445:LEU:H	2.13	0.62
1:A:25:TYR:CD2	1:A:71:VAL:HG22	2.34	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
1:A:255:PHE:CE2	1:A:335:MSE:HE1	2.35	0.61
1:D:380:ILE:HG22	1:D:381:ILE:N	2.14	0.61
1:D:100:VAL:HG12	1:D:106:GLN:HG2	1.80	0.61
1:D:148:ASP:O	1:D:149:ASP:HB2	2.00	0.61
1:A:146:LYS:HB2	1:A:150:THR:HG22	1.82	0.61
2:H:1069:ILE:HD12	2:H:1076:LEU:HD12	1.81	0.61
2:B:1069:ILE:HD12	2:B:1076:LEU:HD12	1.82	0.61
1:A:38:ILE:HD11	1:A:80:LEU:HD13	1.83	0.61
1:A:148:ASP:O	1:A:149:ASP:HB2	2.00	0.61
2:K:1015:PRO:HG2	2:K:1018:SER:OG	1.99	0.61
1:J:380:ILE:HG22	1:J:381:ILE:N	2.15	0.61
1:D:372:LYS:HE2	1:D:385:ASN:ND2	2.16	0.61
1:D:146:LYS:HB2	1:D:150:THR:HG22	1.81	0.61
1:A:380:ILE:HG22	1:A:381:ILE:N	2.14	0.61
1:J:100:VAL:HG12	1:J:106:GLN:HG2	1.83	0.61
1:D:297:TYR:HB3	1:D:320:ASP:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:148:ASP:O	1:G:149:ASP:HB2	2.00	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: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:G:444:THR:CG2	1:G:445:LEU:H	2.13	0.60
1:A:307:ILE:HD11	1:A:314:ILE:HD11	1.84	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:G:38:ILE:HD11	1:G:80:LEU:HD13	1.84	0.60
1:A:297:TYR:HB3	1:A:320:ASP:HB2	1.84	0.60
1:G:146:LYS:HB2	1:G:150:THR:HG22	1.84	0.59
2:K:1065:THR:HG22	2:K:1067:LYS:HG3	1.83	0.59
1:J:372:LYS:HE2	1:J:385:ASN:ND2	2.16	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:D:343:VAL:O	1:D:344:TYR:HB2	2.02	0.59
1:A:100:VAL:HG12	1:A:106:GLN:HG2	1.83	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:G:386:PHE:HB3	1:G:412:SER:OG	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:26:ILE:HB	1:G:440:MSE:HE3	1.86	0.57
2:E:1065:THR:HG22	2:E:1067:LYS:HG3	1.84	0.57
3:I:1437:VAL:CG1	1:J:243:VAL:CG1	2.82	0.57
1:D:444:THR:CG2	1:D:445:LEU:H	2.14	0.57
1:D:402:LEU:HD21	3:F:1448:GLN:HB3	1.84	0.57
1:G:305:ILE:HD12	1:G:305:ILE:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:1452:PHE:CE1	3:L:1456:LEU:HD22	2.39	0.57
1:G:297:TYR:HB3	1:G:320:ASP:HB2	1.85	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
1:J:307:ILE:HD11	1:J:314:ILE:CD1	2.34	0.57
2:B:966:MSE:HG3	2:B:1020:GLY:HA3	1.86	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
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:1081:ILE:HG22	2:B:1085:LYS:HE3	1.85	0.57
1:J:440:MSE:CE	1:J:445:LEU:HD13	2.35	0.56
2:B:983:SER:CB	2:B:986:GLN:HG2	2.35	0.56
1:J:146:LYS:HB2	1:J:150:THR:HG22	1.87	0.56
2:H:1065:THR:HG22	2:H:1067:LYS:HG3	1.87	0.56
3:I:1456:LEU:O	3:I:1456:LEU:HD12	2.05	0.56
1:A:29:SER:OG	1:A:77:GLY:HA3	2.05	0.56
2:E:983:SER:CB	2:E:986:GLN:HG2	2.35	0.56
3:C:1434:PHE:C	3:C:1436:VAL:H	2.08	0.56
1:A:29:SER:HB3	1:A:34:ARG:HD3	1.87	0.56
2:K:1065:THR:HG21	2:K:1067:LYS:HD2	1.88	0.56
2:K:966:MSE:HG3	2:K:1020:GLY:HA3	1.86	0.56
2:H:966:MSE:HG3	2:H:1020:GLY:HA3	1.87	0.56
1:J:305:ILE:HD12	1:J:305:ILE:N	2.21	0.56
2:H:1010:ASP:CB	2:H:1046:GLY:HA2	2.27	0.56
2:E:1065:THR:HG21	2:E:1067:LYS:HD2	1.86	0.56
1:G:82:LEU:HD12	1:G:82:LEU:N	2.21	0.56
2:E:1081:ILE:HG22	2:E:1085:LYS:HE3	1.86	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:J:242:ASP:OD1	1:J:244:ILE:N	2.39	0.56
1:D:257:SER:O	1:D:261:GLU:HG3	2.05	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:J:29:SER:HB3	1:J:34:ARG:HD3	1.87	0.55
1:D:242:ASP:OD1	1:D:244:ILE:N	2.39	0.55
1:A:402:LEU:HD21	3:C:1448:GLN:HB3	1.88	0.55
1:J:29:SER:OG	1:J:77:GLY:HA3	2.06	0.55
2:B:1010:ASP:HB3	2:B:1046:GLY:HA2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:1434:PHE:N	3:F:1434:PHE:CD1	2.73	0.55
2:B:1065:THR:HG21	2:B:1067:LYS:HD2	1.87	0.55
2:H:983:SER:CB	2:H:986:GLN:HG2	2.35	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:K:1041:PRO:HB2	2:K:1048:ASN:HB2	1.88	0.55
1:A:386:PHE:HB3	1:A:412:SER:OG	2.06	0.55
2:H:1065:THR:HG21	2:H:1067:LYS:HD2	1.89	0.55
1:J:381:ILE:HD11	1:J:420:ILE:HG21	1.89	0.55
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
2:E:966:MSE:HG3	2:E:1020:GLY:HA3	1.88	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:D:386:PHE:HB3	1:D:412:SER:OG	2.07	0.54
1:A:210:PRO:HG3	1:A:335:MSE:CE	2.34	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:J:402:LEU:HD21	3:L:1448:GLN:CB	2.38	0.53
1:G:402:LEU:HD21	3:I:1448:GLN:HB3	1.91	0.53
2:K:1017:THR:HG22	2:K:1017:THR:O	2.08	0.53
1:G:332:GLU:CB	3:I:1443:MSE:HE3	2.39	0.53
1:G:10:LEU:HD21	1:G:46:TYR:HE2	1.73	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: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:G:242:ASP:OD1	1:G:244:ILE:N	2.41	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:173:PHE:CZ	2:H:1109:ALA:O	2.62	0.53
1:A:380:ILE:CG2	1:A:381:ILE:N	2.71	0.53
1:A:82:LEU:HD12	1:A:82:LEU:N	2.24	0.53
1:G:199:THR:O	1:G:199:THR:HG22	2.09	0.53
1:A:138:ARG:NH2	1:A:157:LEU:HD13	2.24	0.53
1:D:307:ILE:HD11	1:D:314:ILE:CD1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1000:TYR:C	2:H:1056:PHE:CD2	2.83	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:J:381:ILE:HD11	1:J:424:PRO:CG	2.38	0.52
1:D:402:LEU:HD21	3:F:1448:GLN:CB	2.40	0.52
1:D:82:LEU:HD12	1:D:82:LEU: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:305:ILE:N	1:D:305:ILE:HD12	2.24	0.52
2:E:1037:LEU:N	2:E:1038:PRO:HD3	2.24	0.52
1:D:27:PHE:CZ	1:D:71:VAL:HG23	2.40	0.52
1:D:29:SER:HB3	1:D:34:ARG:HD3	1.90	0.52
1:J:356:LEU:O	1:J:358:ARG:HG3	2.10	0.52
2:B:1017:THR:O	2:B:1017:THR:HG22	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:J:422:ARG:CG	1:J:442:ASN:HD21	2.22	0.51
1:G:381:ILE:HD11	1:G:420:ILE:HG21	1.92	0.51
2:K:1087:ASN:C	2:K:1089:ASN:H	2.13	0.51
1:A:307:ILE:HD11	1:A:314:ILE:CD1	2.40	0.51
1:J:138:ARG:NH2	1:J:157:LEU:HD13	2.25	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:D:440:MSE:CE	1:D:445:LEU:HD13	2.39	0.51
2:K:983:SER:CB	2:K:986:GLN:HG2	2.35	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
1:D:422:ARG:O	1:D:423:ILE:C	2.49	0.51
1:G:27:PHE:CZ	1:G:71:VAL:HG23	2.42	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:J:321:ASP:OD2	1:J:323:SER:HB2	2.09	0.51
1:J:238:ASP:OD2	1:J:240:THR:HB	2.10	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:G:422:ARG:O	1:G:423:ILE:C	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:PRO:CB	1:A:335:MSE:HE3	2.40	0.51
1:J:27:PHE:CZ	1:J:71:VAL:HG23	2.40	0.51
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:A:393:LEU:O	1:A:397:ILE:HG13	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:A:199:THR:O	1:A:199:THR:HG22	2.10	0.50
1:J:199:THR:O	1:J:199:THR:HG22	2.10	0.50
2:H:1009:VAL:HG13	2:H:1046:GLY:O	2.10	0.50
1:D:210:PRO:HG3	1:D:335:MSE:CE	2.39	0.50
1:J:137:TYR:CE2	1:J:138:ARG:HG3	2.46	0.50
1:A:237:LEU:HD22	1:A:246:LYS:HG3	1.93	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:420:ILE:HG21	1:G:424:PRO:HG3	1.94	0.50
1:G:388:SER:OG	1:G:413:LYS:HE3	2.12	0.50
1:J:425:ASN:HB3	1:J:440:MSE:HB3	1.94	0.50
1:A:37:PHE:HE1	1:A:440:MSE:CE	2.25	0.50
1:J:210:PRO:CB	1:J:335:MSE:HE3	2.42	0.50
2:H:1017:THR:HG22	2:H:1017:THR:O	2.12	0.50
2:B:1001:GLY:HA2	2:B:1056:PHE:CE2	2.47	0.50
1:G:381:ILE:HD11	1:G:424:PRO:CG	2.38	0.50
1:A:422:ARG:O	1:A:423:ILE:C	2.50	0.50
1:G:250:ILE:O	1:G:254:GLN:HG3	2.12	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:7:LEU:HB2	1:G:431:TRP:CH2	2.46	0.50
1:A:403:ASN:HB2	1:A:404:PRO:HD3	1.94	0.50
1:J:325:ILE:O	1:J:325:ILE:HG13	2.12	0.49
1:A:446:THR:HG22	1:A:447:PHE:N	2.26	0.49
1:G:167:ASN:O	1:G:178:ARG:NH1	2.43	0.49
1:J:422:ARG:O	1:J:423:ILE:C	2.50	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:G:440:MSE:CE	1:G:445:LEU:HD13	2.40	0.49
2:B:995:VAL:HG21	2:B:1024:ILE:HD12	1.93	0.49
1:A:27:PHE:CZ	1:A:71:VAL:HG23	2.42	0.49
1:A:343:VAL:O	1:A:344:TYR:CB	2.61	0.49
1:G:45:TRP:CZ2	1:G:94:PRO:HB2	2.47	0.49
1:D:199:THR:O	1:D:199:THR:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:425:ASN:HB3	1:G:440:MSE:HB3	1.94	0.49
1:A:425:ASN:HB3	1:A:440:MSE:HB3	1.94	0.49
1:D:356:LEU:O	1:D:358:ARG:HG3	2.13	0.49
1:D:189:LYS:HG2	1:D:304:THR:HG21	1.91	0.49
1:G:30:GLN:CG	1:G:34:ARG:HD2	2.42	0.49
2:E:1018:SER:HB3	2:E:1023:ILE:HG13	1.94	0.49
1:D:212:LEU:HD13	1:D:272:ILE:HD13	1.95	0.49
1:G:240:THR:HG22	1:G:240:THR:O	2.12	0.49
1:A:332:GLU:CB	3:C:1443:MSE:HE3	2.43	0.49
1:G:189:LYS:HG2	1:G:304:THR:HG22	1.94	0.49
1:D:250:ILE:O	1:D:254:GLN:HG3	2.12	0.49
2:E:982:TYR:HB2	2:E:987:LEU:HD13	1.93	0.49
1:J:392:THR:CG2	1:J:408:LEU:HD11	2.41	0.48
1:A:392:THR:CG2	1:A:408:LEU:HD11	2.43	0.48
1:A:167:ASN:O	1:A:178:ARG:NH1	2.46	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:A:444:THR:CG2	1:A:445:LEU:N	2.75	0.48
1:D:210:PRO:CB	1:D:335:MSE:HE3	2.43	0.48
1:D:45:TRP:CE2	1:D:55:HIS:HB2	2.49	0.48
1:J:30:GLN:CG	1:J:34:ARG:HD2	2.44	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
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:A:189:LYS:HG2	1:A:304:THR:HG22	1.95	0.48
3:L:1453:PHE:O	3:L:1457:ASN:ND2	2.43	0.48
1:A:45:TRP:CZ2	1:A:94:PRO:HB2	2.48	0.48
1:J:420:ILE:HG21	1:J:424:PRO:HG3	1.95	0.48
1:G:325:ILE:HG13	1:G:325:ILE:O	2.14	0.48
1:D:133:HIS:CE1	1:D:213:PRO:HD3	2.49	0.48
1:G:451:SER:O	1:G:452:SER:HB3	2.13	0.48
1:G:273:GLN:OE1	1:G:276:TYR:HE1	1.97	0.48
1:J:451:SER:O	1:J:452:SER:HB3	2.13	0.48
1:J:391:SER:O	1:J:395:LYS:HG3	2.14	0.48
3:F:1456:LEU:HG	3:F:1456:LEU:O	2.14	0.48
1:A:61:ARG:NH1	1:A:107:ASP:OD1	2.46	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:D:9:ALA:O	1:D:10:LEU:C	2.52	0.48
1:D:425:ASN:HB3	1:D:440:MSE:HB3	1.95	0.48
1:D:381:ILE:HD11	1:D:424:PRO:CG	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:1038:PRO:C	2:E:1040:ARG:N	2.57	0.48
1:A:422:ARG:CG	1:A:442:ASN:HD21	2.26	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:A:198:ASN:O	1:A:203:GLY:HA2	2.14	0.48
1:D:451:SER:O	1:D:452:SER:HB3	2.13	0.48
1:J:250:ILE:O	1:J:254:GLN:HG3	2.14	0.48
1:J:229:LYS:HE3	1:J:332:GLU:CD	2.34	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
2:H:1036:ASN:O	2:H:1037:LEU:HB2	2.13	0.47
1:D:148:ASP:HB3	1:D:150:THR:CB	2.41	0.47
1:J:361:LYS:O	1:J:362:SER:HB3	2.14	0.47
1:G:391:SER:O	1:G:395:LYS:HG3	2.15	0.47
3:I:1437:VAL:HG12	1:J:243:VAL:CG1	2.45	0.47
1:A:451:SER:O	1:A:452:SER:HB3	2.14	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
1:J:7:LEU:N	1:J:431:TRP:CZ3	2.82	0.47
1:G:396:SER:HB2	1:G:401:ASP:O	2.15	0.47
1:A:37:PHE:HE1	1:A:440:MSE:HE1	1.78	0.47
1:A:33:THR:HG22	1:A:34:ARG:HG3	1.96	0.47
1:G:137:TYR:CE2	1:G:138:ARG:HG3	2.49	0.47
1:J:446:THR:HG22	1:J:447:PHE:N	2.29	0.47
1:A:396:SER:HB2	1:A:401:ASP:O	2.14	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: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: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
1:A:240:THR:O	1:A:241:THR:C	2.54	0.47
1:J:380:ILE:CG2	1:J:382:GLN:HG3	2.45	0.46
1:G:30:GLN:CD	1:G:34:ARG:HD2	2.36	0.46
1:G:45:TRP:CE2	1:G:55:HIS:HB2	2.50	0.46
1:D:388:SER:OG	1:D:413:LYS:HE3	2.15	0.46
1:J:45:TRP:CZ2	1:J:94:PRO:HB2	2.50	0.46
1:G:422:ARG:CG	1:G:442:ASN:HD21	2.26	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:422:ARG:O	1:A:424:PRO:N	2.48	0.46
1:G:343:VAL:HG11	2:H:1066:ARG:CZ	2.45	0.46
3:F:1434:PHE:O	3:F:1436:VAL:N	2.49	0.46
2:K:1034:TYR:CE2	2:K:1041:PRO:HG2	2.51	0.46
1:J:352:GLU:CG	1:J:353:ARG:N	2.78	0.46
1:G:352:GLU:CG	1:G:353:ARG:N	2.78	0.46
1:D:198:ASN:O	1:D:203:GLY:HA2	2.15	0.46
1:G:361:LYS:O	1:G:362:SER:HB3	2.15	0.46
1:G:343:VAL:O	1:G:344:TYR:CB	2.62	0.46
1:D:9:ALA:O	1:D:10:LEU:O	2.33	0.46
1:J:45:TRP:CE2	1:J:55:HIS:HB2	2.50	0.46
1:G:198:ASN:O	1:G:203:GLY:HA2	2.15	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:G:392:THR:CG2	1:G:408:LEU:HD11	2.44	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:A:380:ILE:CG2	1:A:382:GLN:HG3	2.45	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:251:LYS:NZ	4:D:6119:PGE:O2	2.45	0.46
2:H:1018:SER:HB3	2:H:1023:ILE:HG13	1.96	0.46
2:H:1007:GLU:CD	2:H:1049:VAL:HG22	2.36	0.46
1:D:50:THR:HG22	1:D:51:ASP:OD1	2.15	0.46
1:D:273:GLN:OE1	1:D:276:TYR:HE1	1.98	0.46
2:B:1060:PRO:HG3	2:B:1080:HIS:CG	2.50	0.46
1:D:352:GLU:CG	1:D:353:ARG:N	2.78	0.46
1:D:289:PRO:HD2	1:D:350:LEU:HB3	1.98	0.46
2:H:1060:PRO:HG3	2:H:1080:HIS:CG	2.51	0.46
2:E:1090:SER:HB3	2:E:1104:PHE:CD2	2.51	0.46
2:K:1030:THR:HG22	2:K:1031:CYS:N	2.31	0.46
1:G:120:GLU:HG3	1:G:120:GLU:H	1.47	0.46
2:H:1040:ARG:N	2:H:1041:PRO:HD3	2.30	0.46
1:A:212:LEU:HD13	1:A:272:ILE:HD13	1.98	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
1:J:210:PRO:HB3	1:J:335:MSE:HE3	1.97	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
2:K:1018:SER:HB3	2:K:1023:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:422:ARG:O	1:G:424:PRO:N	2.49	0.45
2:B:972:ILE:HG12	2:B:995:VAL:HG22	1.97	0.45
1:A:137:TYR:CE2	1:A:138:ARG:HG3	2.51	0.45
1:A:45:TRP:CE2	1:A:55:HIS:HB2	2.52	0.45
2:E:1030:THR:HG22	2:E:1031:CYS:N	2.32	0.45
1:J:273:GLN:OE1	1:J:276:TYR:HE1	1.99	0.45
1:G:307:ILE:CG2	1:G:394:SER:HB3	2.47	0.45
2:K:1015:PRO:O	2:K:1017:THR:N	2.50	0.45
1:J:198:ASN:O	1:J:203:GLY:HA2	2.16	0.45
1:A:135:LYS:HD2	1:A:191:GLY:HA3	1.98	0.45
1:A:325:ILE:O	1:A:325:ILE:HG13	2.15	0.45
1:J:189:LYS:HG2	1:J:304:THR:HG21	1.95	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:7:LEU:C	1:J:9:ALA:H	2.20	0.45
1:J:61:ARG:NH1	1:J:107:ASP:OD1	2.49	0.45
1:J:422:ARG:O	1:J:424:PRO:N	2.49	0.45
1:G:173:PHE:CE2	2:H:1033:ILE:HD12	2.45	0.45
2:K:1037:LEU:H	2:K:1038:PRO:HD3	1.80	0.45
2:B:1040:ARG:N	2:B:1041:PRO:CD	2.80	0.45
1:J:321:ASP:CG	1:J:323:SER:HB2	2.37	0.45
1:A:352:GLU:CG	1:A:353:ARG:N	2.79	0.45
2:H:1041:PRO:HB2	2:H:1048:ASN:HB2	1.99	0.45
1:A:368:GLU:HG2	1:A:428:TYR:CE2	2.51	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
1:J:212:LEU:HD13	1:J:272:ILE:HD13	1.98	0.45
1:D:361:LYS:O	1:D:362:SER:HB3	2.16	0.45
1:J:307:ILE:CG2	1:J:394:SER:HB3	2.47	0.45
2:B:1009:VAL:HG13	2:B:1046:GLY:O	2.17	0.45
1:D:368:GLU:HG2	1:D:428:TYR:CE2	2.52	0.45
1:J:210:PRO:HG3	1:J:335:MSE:CE	2.42	0.45
1:A:15:ALA:HB2	1:A:24:ARG:NH2	2.31	0.45
1:A:307:ILE:HG12	1:A:390:ALA:HB1	1.98	0.45
1:J:82:LEU:HD12	1:J:82:LEU:H	1.81	0.45
1:D:202:GLY:HA2	2:E:1079:ARG:NH1	2.32	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
2:H:972:ILE:HD11	2:H:1019:LEU:CB	2.43	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
1:J:30:GLN:HG3	1:J:34:ARG:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1029:LYS:HE2	2:H:1058:CYS:HA	2.00	0.44
1:A:328:PHE:HB2	1:A:351:ILE:HD11	1.99	0.44
2:H:1030:THR:HG22	2:H:1031:CYS:N	2.31	0.44
1:D:30:GLN:CG	1:D:34:ARG:HD2	2.47	0.44
1:J:199:THR:CG2	1:J:199:THR:O	2.64	0.44
2:K:1060:PRO:HG3	2:K:1080:HIS:CD2	2.53	0.44
1:G:239:SER:C	1:G:241:THR:H	2.21	0.44
1:J:380:ILE:HG21	1:J:382:GLN:HG3	2.00	0.44
1:G:380:ILE:CG2	1:G:382:GLN:HG3	2.48	0.44
1:D:307:ILE:CG2	1:D:394:SER:HB3	2.48	0.44
1:J:368:GLU:HG2	1:J:428:TYR:CE2	2.52	0.44
1:G:148:ASP:HB3	1:G:150:THR:CB	2.43	0.44
1:J:30:GLN:CD	1:J:34:ARG:HD2	2.38	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:D:188:SER:HB3	1:D:190:ASP:OD1	2.18	0.44
2:B:1034:TYR:CE2	2:B:1041:PRO:HG2	2.52	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
1:D:167:ASN:O	1:D:178:ARG:NH1	2.51	0.44
1:A:210:PRO:HB3	1:A:335:MSE:HE3	1.99	0.44
1:A:78:ASP:O	1:A:79:LEU:HD23	2.18	0.44
1:D:102:ASP:HB3	1:D:105:ILE:H	1.82	0.44
1:A:273:GLN:OE1	1:A:276:TYR:HE1	2.00	0.44
2:E:1049:VAL:HG13	2:E:1050:ARG:N	2.33	0.44
3:C:1450:GLY:O	3:C:1454:LYS:HG3	2.18	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:D:30:GLN:HG3	1:D:34:ARG:HD2	2.00	0.43
1:A:199:THR:O	1:A:199:THR:CG2	2.65	0.43
1:J:102:ASP:HB3	1:J:105:ILE:H	1.83	0.43
1:D:61:ARG:NH1	1:D:107:ASP:OD1	2.49	0.43
1:G:210:PRO:CB	1:G:335:MSE:HE3	2.48	0.43
1:A:30:GLN:CG	1:A:34:ARG:HD2	2.48	0.43
1:D:358:ARG:NH2	1:D:380:ILE:HD12	2.33	0.43
1:G:229:LYS:HE3	1:G:332:GLU:CD	2.39	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:A:381:ILE:O	1:A:417:ILE:HB	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:307:ILE:HG12	1:J:390:ALA:HB1	2.01	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:G:289:PRO:HD2	1:G:350:LEU:HB3	2.00	0.43
1:A:391:SER:O	1:A:395:LYS:HG3	2.18	0.43
1:G:381:ILE:O	1:G:417:ILE:HB	2.17	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:CG2	1:G:199:THR:O	2.65	0.43
2:H:1047:ILE:O	2:H:1047:ILE:HG22	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
1:G:102:ASP:HB3	1:G:105:ILE:H	1.84	0.43
2:E:968:GLU:HG3	2:E:968:GLU:H	1.45	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
1:A:316:CYS:SG	1:A:324:LEU:HG	2.59	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:J:386:PHE:HB2	1:J:389:TRP:CE2	2.54	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
3:I:1452:PHE:C	3:I:1452:PHE:CD1	2.92	0.43
1:J:381:ILE:O	1:J:417:ILE:HB	2.18	0.42
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: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
3:L:1452:PHE:C	3:L:1452:PHE:CD1	2.92	0.42
1:J:238:ASP:OD2	1:J:240:THR:CB	2.68	0.42
1:D:199:THR:O	1:D:200:THR:C	2.56	0.42
1:J:451:SER:O	1:J:452:SER:CB	2.67	0.42
1:D:10:LEU:HA	1:D:11:PRO:HD3	1.93	0.42
1:A:321:ASP:OD2	1:A:353:ARG:NH2	2.52	0.42
1:A:212:LEU:O	1:A:277:ARG:HD2	2.18	0.42
1:D:328:PHE:HB2	1:D:351:ILE:HD11	2.01	0.42
1:J:159:SER:C	1:J:161:GLU:H	2.22	0.42
1:A:102:ASP:HB3	1:A:105:ILE:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:440:MSE:HB2	1:J:440:MSE:HE2	1.98	0.42
1:G:252:GLN:HG3	1:G:335:MSE:SE	2.69	0.42
2:E:1037:LEU:N	2:E:1038:PRO:CD	2.82	0.42
2:E:972:ILE:HG12	2:E:995:VAL:HG22	1.99	0.42
1:D:274:LYS:HG3	1:D:275:GLU:OE2	2.20	0.42
1:J:358:ARG:NH2	1:J:380:ILE:HD12	2.33	0.42
1:J:148:ASP:HB3	1:J:150:THR:CB	2.43	0.42
1:G:247:ARG:NH1	1:G:338:ASP:OD2	2.50	0.42
2:K:1065:THR:HG22	2:K:1067:LYS:CG	2.49	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:316:CYS:SG	1:D:324:LEU:HG	2.59	0.42
3:C:1452:PHE:C	3:C:1452:PHE:CD1	2.92	0.42
1:D:135:LYS:HD2	1:D:191:GLY:HA3	2.01	0.42
1:D:159:SER:C	1:D:161:GLU:H	2.23	0.42
1:J:135:LYS:HD2	1:J:191:GLY:HA3	2.02	0.42
1:D:276:TYR:CD2	4:D:6119:PGE:H5	2.53	0.42
3:F:1434:PHE:C	3:F:1436:VAL:H	2.23	0.42
2:E:1079:ARG:O	2:E:1083:ARG:HG2	2.20	0.42
1:J:199:THR:O	1:J:200:THR:C	2.58	0.42
1:A:120:GLU:HG3	1:A:120:GLU:H	1.47	0.42
1:A:358:ARG:NH2	1:A:380:ILE:HD12	2.34	0.42
1:G:386:PHE:HB2	1:G:389:TRP:CE2	2.54	0.42
1:D:199:THR:CG2	1:D:199:THR:O	2.68	0.42
1:J:50:THR:HG22	1:J:51:ASP:OD1	2.20	0.42
1:D:325:ILE:O	1:D:325:ILE:HG13	2.18	0.42
3:F:1450:GLY:O	3:F:1454:LYS:HG3	2.20	0.42
2:E:1010:ASP:HB3	2:E:1046:GLY:HA2	2.02	0.42
1:A:290:PHE:HA	1:A:291:PRO:HD3	1.86	0.42
1:J:343:VAL:CG1	2:K:1066:ARG:CZ	2.95	0.42
2:E:972:ILE:CG2	2:E:973:SER:N	2.83	0.42
1:J:28:SER:HA	1:J:34:ARG:O	2.19	0.42
1:G:28:SER:HA	1:G:34:ARG:O	2.19	0.42
2:E:1015:PRO:O	2:E:1017:THR:N	2.52	0.42
1:G:82:LEU:HD12	1:G:82:LEU:H	1.84	0.42
2:H:972:ILE:HG12	2:H:995:VAL:HG22	2.02	0.42
1:G:358:ARG:NH2	1:G:380:ILE:HD12	2.34	0.42
2:K:972:ILE:CG2	2:K:973:SER:N	2.82	0.42
1:A:288:ASN:O	1:A:349:VAL:HA	2.20	0.42
1:A:239:SER:HA	1:A:246:LYS:NZ	2.34	0.42
1:D:10:LEU:HG	1:D:11:PRO:HD2	2.02	0.42
1:A:213:PRO:O	1:A:277:ARG:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:43:ILE:O	1:D:56:SER:HA	2.19	0.42
1:D:380:ILE:HG21	1:D:382:GLN:HG3	2.01	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
1:J:168:LYS:O	1:J:178:ARG:HD3	2.20	0.41
1:A:50:THR:HG22	1:A:51:ASP:OD1	2.19	0.41
1:A:15:ALA:HB2	1:A:39:GLN:OE1	2.19	0.41
1:J:33:THR:HG22	1:J:34:ARG:HG3	2.01	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:H:1054:THR:HG23	2:H:1103:VAL:HG22	2.01	0.41
2:B:1079:ARG:O	2:B:1083:ARG:HG2	2.20	0.41
1:G:50:THR:HG22	1:G:51:ASP:OD1	2.21	0.41
3:C:1437:VAL:O	3:C:1441:LEU:HG	2.21	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:159:SER:C	1:A:161:GLU:H	2.24	0.41
1:A:252:GLN:HG3	1:A:335:MSE:SE	2.70	0.41
2:E:1039:ASN:O	2:E:1040:ARG:C	2.58	0.41
2:B:966:MSE:HE2	2:B:1020:GLY:CA	2.50	0.41
2:K:966:MSE:HE2	2:K:1020:GLY:CA	2.50	0.41
2:H:966:MSE:HE2	2:H:1020:GLY:CA	2.51	0.41
1:D:451:SER:O	1:D:452:SER:CB	2.68	0.41
1:J:213:PRO:O	1:J:277:ARG:HD3	2.20	0.41
1:G:159:SER:C	1:G:161:GLU:H	2.22	0.41
2:E:1006:LEU:HD21	2:E:1052:ARG:NH1	2.35	0.41
1:G:440:MSE:HE2	1:G:440:MSE:HB2	2.00	0.41
1:G:210:PRO:CD	1:G:335:MSE:HE3	2.50	0.41
1:D:381:ILE:O	1:D:417:ILE:HB	2.20	0.41
1:G:189:LYS:NZ	1:G:304:THR:HG22	2.36	0.41
1:G:30:GLN:HB2	1:G:33:THR:HG22	2.02	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:302:ILE:HA	1:A:316:CYS:O	2.21	0.41
1:G:212:LEU:O	1:G:277:ARG:HD2	2.21	0.41
2:E:1061:VAL:CG1	2:E:1066:ARG:HA	2.51	0.41
1:J:252:GLN:HG3	1:J:335:MSE:SE	2.71	0.41
1:D:137:TYR:CD2	1:D:138:ARG:HG3	2.56	0.41
2:H:1030:THR:CG2	2:H:1031:CYS:N	2.83	0.41
1:G:43:ILE:O	1:G:56:SER:HA	2.20	0.41
1:D:252:GLN:HG3	1:D:335:MSE:SE	2.71	0.41
1:J:93:VAL:HA	1:J:94:PRO:HD3	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:133:HIS:HA	1:G:134:PRO:HD3	1.93	0.41
2:E:1060:PRO:HG3	2:E:1080:HIS:CD2	2.56	0.41
2:B:972:ILE:CG2	2:B:973:SER:N	2.83	0.41
1:A:30:GLN:CD	1:A:34:ARG:HD2	2.40	0.41
2:H:1015:PRO:O	2:H:1017:THR:N	2.54	0.41
1:J:386:PHE:HB2	1:J:389:TRP:CZ2	2.55	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CE2	2.55	0.41
1:G:402:LEU:HD21	3:I:1448:GLN:CB	2.50	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:G:321:ASP:OD2	1:G:353:ARG:NH2	2.54	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:A:7:LEU:HG	1:A:9:ALA:HB3	2.02	0.41
2:E:1084:LEU:C	2:E:1086:LYS:H	2.23	0.41
1:J:26:ILE:HB	1:J:440:MSE:HE3	2.03	0.41
1:D:444:THR:CG2	1:D:445:LEU:N	2.74	0.41
2:H:1000:TYR:C	2:H:1056:PHE:HD2	2.22	0.41
2:K:1087:ASN:O	2:K:1087:ASN:CG	2.60	0.41
1:J:332:GLU:HG2	3:L:1443:MSE:HE3	2.01	0.41
1:A:239:SER:HA	1:A:246:LYS:HZ1	1.86	0.41
3:F:1452:PHE:CD1	3:F:1452:PHE:C	2.93	0.41
1:A:451:SER:O	1:A:452:SER:CB	2.68	0.41
2:K:1030:THR:CG2	2:K:1031:CYS:N	2.82	0.41
1:J:133:HIS:HA	1:J:134:PRO:HD3	1.92	0.41
1:A:291:PRO:HB2	1:A:294:LEU:HD12	2.03	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CZ2	2.56	0.41
1:J:137:TYR:CD2	1:J:138:ARG:HG3	2.56	0.41
1:D:168:LYS:O	1:D:178:ARG:HD3	2.21	0.41
2:K:1054:THR:HG23	2:K:1103:VAL:HG22	2.03	0.41
1:J:274:LYS:HG3	1:J:275:GLU:OE2	2.20	0.41
1:G:291:PRO:HB2	1:G:294:LEU:HD12	2.02	0.41
1:G:290:PHE:HA	1:G:291:PRO:HD3	1.86	0.41
1:D:240:THR:OG1	1:G:9:ALA:HB2	2.21	0.41
1:D:251:LYS:HB3	4:D:6119:PGE:H62	2.03	0.40
1:J:210:PRO:HB2	1:J:212:LEU:HG	2.03	0.40
1:A:372:LYS:HE2	1:A:385:ASN:HD21	1.84	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
2:B:1047:ILE:HG22	2:B:1047:ILE:O	2.20	0.40
1:A:228:ASN:ND2	3:C:1435:LYS:HB2	2.36	0.40
2:E:1036:ASN:O	2:E:1037:LEU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:386:PHE:HB2	1:G:389:TRP:CZ2	2.55	0.40
2:H:966:MSE:HG3	2:H:1020:GLY:CA	2.50	0.40
1:J:321:ASP:OD2	1:J:353:ARG:NH2	2.54	0.40
1:G:321:ASP:CG	1:G:323:SER:HB2	2.41	0.40
1:J:302:ILE:HA	1:J:316:CYS:O	2.21	0.40
2:K:988:ARG:HA	2:K:1010:ASP:HA	2.02	0.40
2:B:1038:PRO:C	2:B:1040:ARG:H	2.24	0.40
1:A:321:ASP:CG	1:A:323:SER:HB2	2.41	0.40
1:J:290:PHE:HA	1:J:291:PRO:HD3	1.85	0.40
2:E:1047:ILE:O	2:E:1047:ILE:HG22	2.20	0.40
1:D:179:VAL:HG21	1:D:281:VAL:HG11	2.04	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
2:H:1061:VAL:CG1	2:H:1066:ARG:HA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	25	49
1	D	431/452 (95%)	397 (92%)	29 (7%)	5 (1%)	19	39
1	G	432/452 (96%)	396 (92%)	32 (7%)	4 (1%)	25	49
1	J	433/452 (96%)	399 (92%)	29 (7%)	5 (1%)	19	39
2	B	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	6	8
2	E	144/148 (97%)	117 (81%)	20 (14%)	7 (5%)	3	4
2	H	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	8	12
2	K	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	6	8
3	C	24/36 (67%)	21 (88%)	2 (8%)	1 (4%)	4	5
3	F	24/36 (67%)	21 (88%)	3 (12%)	0	100	100
3	I	26/36 (72%)	25 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

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%)	14	26

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

Continued on next page...

Continued from previous page...

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%)	396 (96%)	15 (4%)	47	76
1	D	410/415 (99%)	398 (97%)	12 (3%)	55	83
1	G	411/415 (99%)	398 (97%)	13 (3%)	51	80
1	J	412/415 (99%)	400 (97%)	12 (3%)	55	83
2	B	132/133 (99%)	128 (97%)	4 (3%)	53	82
2	E	132/133 (99%)	128 (97%)	4 (3%)	53	82
2	H	132/133 (99%)	128 (97%)	4 (3%)	53	82
2	K	132/133 (99%)	128 (97%)	4 (3%)	53	82
3	C	22/28 (79%)	22 (100%)	0	100	100
3	F	22/28 (79%)	21 (96%)	1 (4%)	38	67
3	I	24/28 (86%)	22 (92%)	2 (8%)	16	30
3	L	21/28 (75%)	21 (100%)	0	100	100
All	All	2261/2304 (98%)	2190 (97%)	71 (3%)	52	81

All (71) 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	101	GLU
1	A	102	ASP
1	A	120	GLU
1	A	148	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	176	ASP
1	A	185	LEU
1	A	198	ASN
1	A	210	PRO
1	A	217	LEU
1	A	281	VAL
1	A	286	THR
1	A	433	ASP
2	B	968	GLU
2	B	1049	VAL
2	B	1079	ARG
2	B	1098	ASP
1	D	29	SER
1	D	33	THR
1	D	101	GLU
1	D	102	ASP
1	D	120	GLU
1	D	148	ASP
1	D	185	LEU
1	D	198	ASN
1	D	210	PRO
1	D	217	LEU
1	D	281	VAL
1	D	286	THR
2	E	968	GLU
2	E	1049	VAL
2	E	1079	ARG
2	E	1098	ASP
3	F	1434	PHE
1	G	29	SER
1	G	33	THR
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	198	ASN
1	G	210	PRO
1	G	217	LEU
1	G	281	VAL
1	G	286	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	968	GLU
2	H	1049	VAL
2	H	1079	ARG
2	H	1098	ASP
3	I	1430	ASP
3	I	1456	LEU
1	J	29	SER
1	J	33	THR
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
2	K	968	GLU
2	K	1049	VAL
2	K	1079	ARG
2	K	1098	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	430	ASN
2	B	967	ASN
2	B	969	ASN
2	B	1075	GLN
2	B	1087	ASN
1	D	262	ASN
1	D	430	ASN
2	E	967	ASN
2	E	969	ASN
2	E	1075	GLN
3	F	1457	ASN
1	G	262	ASN
2	H	967	ASN
2	H	969	ASN
3	I	1448	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	262	ASN
2	K	967	ASN
2	K	969	ASN
2	K	1075	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	0.91	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	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6119	PGE	C5-C6	2.17	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/452 (96%)	0.18	11 (2%) 54 52	44, 65, 98, 118	0
1	D	437/452 (96%)	0.16	7 (1%) 68 69	41, 65, 98, 118	0
1	G	438/452 (96%)	0.13	10 (2%) 57 54	43, 65, 98, 117	0
1	J	439/452 (97%)	0.15	12 (2%) 52 49	41, 64, 99, 117	0
2	B	146/148 (98%)	0.49	9 (6%) 20 17	53, 90, 119, 129	0
2	E	146/148 (98%)	0.42	10 (6%) 17 14	52, 90, 117, 129	0
2	H	146/148 (98%)	1.84	60 (41%) 1 0	58, 94, 122, 144	0
2	K	146/148 (98%)	0.75	19 (13%) 4 3	56, 92, 121, 137	0
3	C	26/36 (72%)	0.24	1 (3%) 38 35	59, 71, 95, 130	0
3	F	26/36 (72%)	0.43	1 (3%) 38 35	58, 70, 96, 128	0
3	I	28/36 (77%)	0.29	2 (7%) 16 12	57, 71, 120, 129	0
3	L	24/36 (66%)	0.04	0 100 100	62, 72, 89, 96	0
All	All	2440/2544 (95%)	0.33	142 (5%) 22 19	41, 71, 107, 144	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1038	PRO	8.1
2	K	1037	LEU	7.7
2	H	1036	ASN	7.6
2	H	1037	LEU	7.3
2	H	966	MSE	7.2
1	A	452	SER	7.0
2	H	1039	ASN	6.9
2	H	1019	LEU	6.3
2	B	1037	LEU	6.2
2	H	986	GLN	6.0
2	H	1034	TYR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	985	LEU	5.5
2	E	1037	LEU	5.4
2	H	1012	ALA	5.3
2	K	982	TYR	5.1
2	H	982	TYR	4.8
2	K	1038	PRO	4.6
2	H	974	PRO	4.6
3	C	1458	MSE	4.5
1	D	421	GLU	4.5
2	H	1040	ARG	4.5
2	H	1018	SER	4.4
2	K	985	LEU	4.4
2	H	1047	ILE	4.3
2	H	1072	PRO	4.2
2	H	1017	THR	4.2
2	K	966	MSE	4.2
1	D	452	SER	4.1
2	H	989	LYS	4.1
2	H	1011	LEU	4.1
2	B	984	LEU	4.0
2	H	1023	ILE	3.9
1	G	452	SER	3.9
2	H	972	ILE	3.9
1	J	452	SER	3.9
2	H	988	ARG	3.7
2	H	1074	HIS	3.6
1	D	443	LYS	3.6
2	K	1047	ILE	3.6
2	H	1044	GLY	3.5
2	H	1016	LEU	3.5
1	A	175	LEU	3.5
2	E	1038	PRO	3.4
1	J	160	GLN	3.4
2	H	1000	TYR	3.3
2	E	1076	LEU	3.3
2	K	1039	ASN	3.3
2	H	984	LEU	3.3
2	K	1034	TYR	3.2
1	D	423	ILE	3.2
2	B	1076	LEU	3.2
2	H	1076	LEU	3.2
2	H	1041	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	979	LEU	3.1
1	A	160	GLN	3.1
1	A	424	PRO	3.1
2	H	1014	ILE	3.1
2	H	1059	TYR	3.0
1	G	443	LYS	3.0
1	G	160	GLN	3.0
2	H	970	TYR	2.9
2	H	969	ASN	2.9
2	H	1098	ASP	2.9
2	H	1111	GLU	2.9
2	K	1040	ARG	2.9
2	H	1035	ALA	2.9
2	H	1045	GLU	2.9
1	J	408	LEU	2.8
2	K	981	SER	2.8
3	F	1458	MSE	2.8
2	H	983	SER	2.8
2	K	1011	LEU	2.8
2	E	966	MSE	2.8
1	A	443	LYS	2.8
2	H	971	TYR	2.7
2	K	1036	ASN	2.7
1	J	409	LYS	2.7
2	K	1042	LYS	2.7
2	E	1097	ALA	2.7
2	E	1089	ASN	2.7
2	H	1022	VAL	2.7
2	K	983	SER	2.6
1	G	407	GLY	2.6
1	G	176	ASP	2.6
2	H	1001	GLY	2.6
2	E	984	LEU	2.6
2	H	1013	GLY	2.6
2	H	977	ASP	2.6
2	H	1015	PRO	2.6
1	J	120	GLU	2.6
2	H	1028	PRO	2.5
1	J	161	GLU	2.5
2	E	1098	ASP	2.5
2	H	1025	THR	2.5
2	E	1016	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	973	SER	2.5
1	D	433	ASP	2.5
2	B	1047	ILE	2.4
2	K	1074	HIS	2.4
2	H	1042	LYS	2.4
1	A	103	VAL	2.4
2	H	1056	PHE	2.4
1	J	176	ASP	2.4
1	G	162	LYS	2.4
1	A	240	THR	2.4
2	H	967	ASN	2.3
1	J	402	LEU	2.3
1	J	405	LEU	2.3
1	J	100	VAL	2.3
2	B	1040	ARG	2.3
1	G	402	LEU	2.3
2	H	1043	ARG	2.3
1	A	423	ILE	2.3
2	H	981	SER	2.3
2	K	1014	ILE	2.2
1	J	123	PRO	2.2
2	H	1110	ALA	2.2
1	G	173	PHE	2.2
1	D	444	THR	2.2
1	A	176	ASP	2.2
1	J	171	ASN	2.2
3	I	1431	MSE	2.2
2	B	1038	PRO	2.2
2	H	1024	ILE	2.1
1	G	120	GLU	2.1
2	H	1029	LYS	2.1
2	B	966	MSE	2.1
2	H	979	LEU	2.1
2	K	987	LEU	2.1
2	H	987	LEU	2.1
2	H	1097	ALA	2.1
3	I	1429	LYS	2.1
2	H	1077	VAL	2.1
1	A	433	ASP	2.0
1	D	105	ILE	2.0
1	G	100	VAL	2.0
2	B	1074	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	1055	CYS	2.0
2	B	1098	ASP	2.0
2	E	989	LYS	2.0
2	K	1016	LEU	2.0
1	A	120	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PGE	D	6119	10/10	0.29	3.00	70,72,77,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.