



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:43 PM UTC

PDB ID : 2OAQ / pdb_00002oaq
Title : Crystal structure of the archaeal secretion ATPase GspE in complex with phosphate
Authors : Yamagata, A.; Tainer, J.A.
Deposited on : 2006-12-17
Resolution : 3.15 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

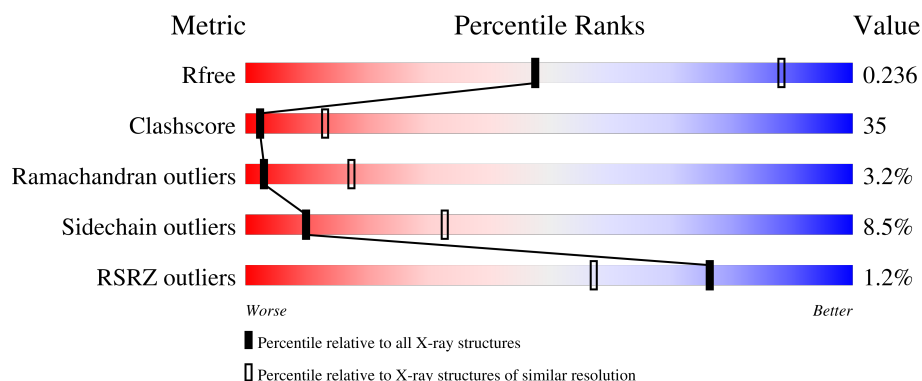
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

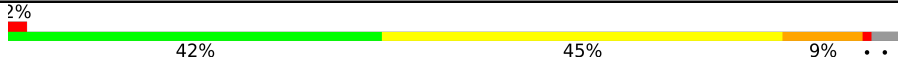
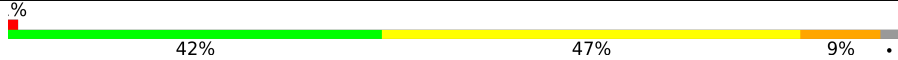
The reported resolution of this entry is 3.15 Å.

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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	1	511	
1	2	511	

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
2	PO4	2	512	-	-	X	-
2	PO4	2	513	-	-	X	-
2	PO4	2	514	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7997 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 Type II secretion system protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	498	Total	C	N	O	S	Se	0	0	0
			3916	2501	669	728	1	17			
1	2	503	Total	C	N	O	S	Se	0	0	0
			4061	2593	681	770	1	16			

There are 36 discrepancies between the modelled and reference sequences:

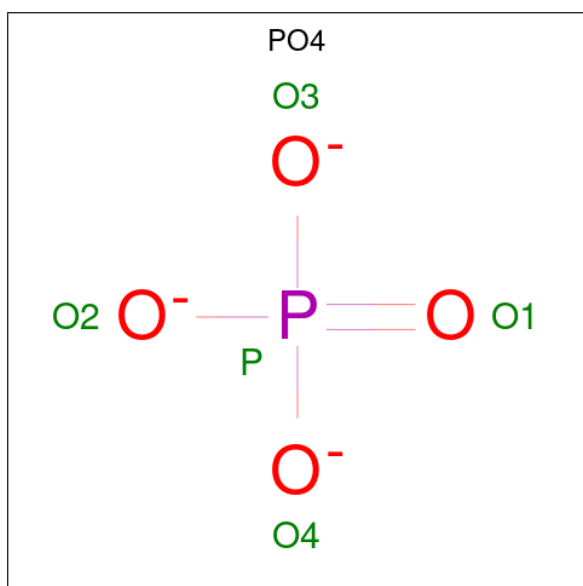
Chain	Residue	Modelled	Actual	Comment	Reference
1	1	MSE	MET	modified residue	UNP O29598
1	121	MSE	MET	modified residue	UNP O29598
1	139	MSE	MET	modified residue	UNP O29598
1	180	MSE	MET	modified residue	UNP O29598
1	281	MSE	MET	modified residue	UNP O29598
1	282	MSE	MET	modified residue	UNP O29598
1	315	MSE	MET	modified residue	UNP O29598
1	322	MSE	MET	modified residue	UNP O29598
1	354	MSE	MET	modified residue	UNP O29598
1	372	MSE	MET	modified residue	UNP O29598
1	387	MSE	MET	modified residue	UNP O29598
1	399	MSE	MET	modified residue	UNP O29598
1	446	MSE	MET	modified residue	UNP O29598
1	453	MSE	MET	modified residue	UNP O29598
1	468	MSE	MET	modified residue	UNP O29598
1	478	MSE	MET	modified residue	UNP O29598
1	504	MSE	MET	modified residue	UNP O29598
1	507	MSE	MET	modified residue	UNP O29598
2	1	MSE	MET	modified residue	UNP O29598
2	121	MSE	MET	modified residue	UNP O29598
2	139	MSE	MET	modified residue	UNP O29598
2	180	MSE	MET	modified residue	UNP O29598
2	281	MSE	MET	modified residue	UNP O29598
2	282	MSE	MET	modified residue	UNP O29598
2	315	MSE	MET	modified residue	UNP O29598

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2	322	MSE	MET	modified residue	UNP O29598
2	354	MSE	MET	modified residue	UNP O29598
2	372	MSE	MET	modified residue	UNP O29598
2	387	MSE	MET	modified residue	UNP O29598
2	399	MSE	MET	modified residue	UNP O29598
2	446	MSE	MET	modified residue	UNP O29598
2	453	MSE	MET	modified residue	UNP O29598
2	468	MSE	MET	modified residue	UNP O29598
2	478	MSE	MET	modified residue	UNP O29598
2	504	MSE	MET	modified residue	UNP O29598
2	507	MSE	MET	modified residue	UNP O29598

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

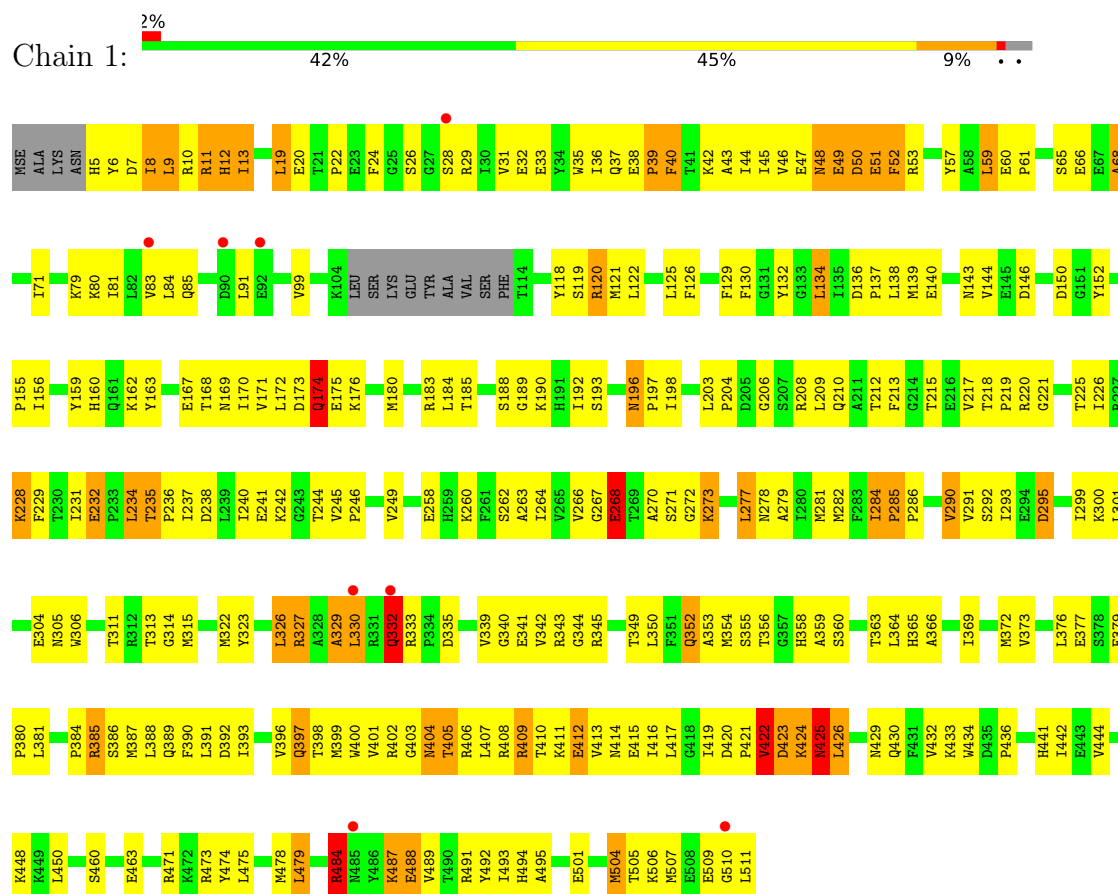


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		

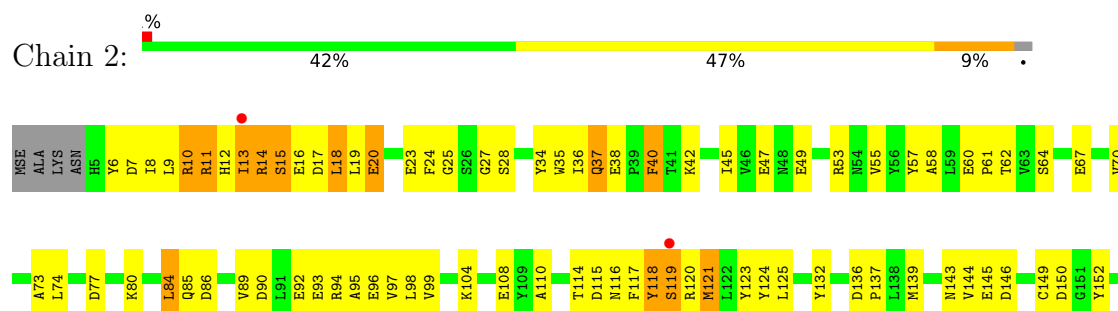
3 Residue-property plots

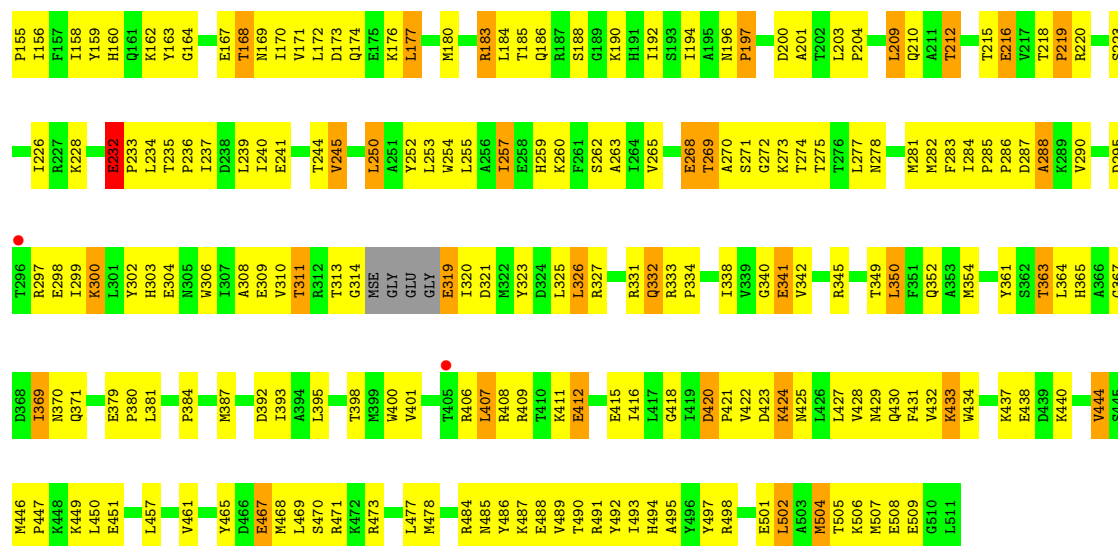
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Type II secretion system protein



• Molecule 1: Type II secretion system protein





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	132.61 Å 132.61 Å 445.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-3.15) 93.2 (20.00-3.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.19 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.236 0.218 , 0.236	Depositor DCC
R_{free} test set	1248 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7997	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1	0.59	2/3977 (0.1%)	1.08	26/5365 (0.5%)
1	2	0.55	0/4125	1.07	26/5560 (0.5%)
All	All	0.57	2/8102 (0.0%)	1.08	52/10925 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	327	ARG	N-CA	6.93	1.55	1.46
1	1	270	ALA	CA-CB	6.38	1.63	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	330	LEU	N-CA-C	-10.55	99.58	111.82
1	1	404	ASN	N-CA-C	-10.42	100.52	113.02
1	1	335	ASP	N-CA-C	-8.91	100.72	111.69
1	2	36	ILE	N-CA-C	-8.37	102.71	111.58
1	1	424	LYS	N-CA-C	-8.03	93.70	110.80
1	2	232	GLU	CA-C-N	7.58	128.77	119.98
1	2	232	GLU	C-N-CA	7.58	128.77	119.98
1	2	408	ARG	N-CA-C	-7.51	96.99	109.46
1	2	27	GLY	N-CA-C	-7.33	105.11	115.30
1	2	260	LYS	N-CA-C	6.76	120.82	111.90
1	1	9	LEU	N-CA-C	-6.66	99.40	109.79
1	2	332	GLN	CB-CA-C	-6.60	106.15	114.40
1	1	150	ASP	N-CA-C	6.54	118.20	111.14
1	2	197	PRO	N-CA-C	6.51	123.05	114.27
1	2	150	ASP	N-CA-C	6.43	119.10	111.71
1	1	210	GLN	N-CA-C	-6.34	99.96	110.17
1	2	285	PRO	CA-C-N	6.33	127.75	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	285	PRO	C-N-CA	6.33	127.75	119.84
1	1	494	HIS	N-CA-C	-6.27	104.44	111.28
1	1	352	GLN	N-CA-C	-6.27	104.53	111.36
1	1	333	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	2	420	ASP	CA-C-N	6.16	125.86	119.82
1	2	420	ASP	C-N-CA	6.16	125.86	119.82
1	1	423	ASP	N-CA-C	6.13	123.87	110.80
1	2	118	TYR	N-CA-C	-6.09	103.38	111.24
1	1	422	VAL	N-CA-C	-6.09	96.68	109.34
1	1	412	GLU	N-CA-C	6.05	118.36	108.55
1	1	425	ASN	N-CA-C	6.02	123.62	110.80
1	2	196	ASN	CA-C-N	5.90	126.41	120.04
1	2	196	ASN	C-N-CA	5.90	126.41	120.04
1	1	12	HIS	N-CA-C	-5.80	106.16	113.18
1	2	121	MSE	N-CA-C	-5.76	105.08	111.36
1	1	196	ASN	CA-C-N	5.75	125.37	119.56
1	1	196	ASN	C-N-CA	5.75	125.37	119.56
1	1	232	GLU	CA-C-N	5.65	125.94	119.83
1	1	232	GLU	C-N-CA	5.65	125.94	119.83
1	1	285	PRO	CA-C-N	5.57	126.80	119.84
1	1	285	PRO	C-N-CA	5.57	126.80	119.84
1	2	304	GLU	N-CA-C	5.57	117.04	110.97
1	2	95	ALA	N-CA-C	-5.47	106.10	112.89
1	2	486	TYR	N-CA-C	5.46	116.92	111.07
1	2	237	ILE	N-CA-C	-5.35	105.50	110.53
1	2	7	ASP	N-CA-C	-5.23	105.66	111.36
1	1	333	ARG	CA-CB-CG	-5.18	103.74	114.10
1	2	286	PRO	N-CA-C	5.17	123.11	112.47
1	1	484	ARG	N-CA-C	5.10	119.50	113.12
1	2	370	ASN	N-CA-C	-5.06	105.66	111.07
1	1	284	ILE	CA-C-N	5.05	125.58	120.38
1	1	284	ILE	C-N-CA	5.05	125.58	120.38
1	1	66	GLU	N-CA-C	-5.04	105.49	111.69
1	2	219	PRO	N-CA-C	-5.02	104.19	111.22
1	2	412	GLU	N-CA-C	5.01	116.03	108.46

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	1	3916	0	3816	287	0
1	2	4061	0	4040	285	0
2	1	5	0	0	1	0
2	2	15	0	0	9	0
All	All	7997	0	7856	561	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 35.

All (561) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:180:MSE:HE2	1:1:184:LEU:HG	1.43	0.99
1:2:446:MSE:HG2	1:2:447:PRO:HD2	1.42	0.98
1:1:215:THR:HG22	1:1:221:GLY:HA2	1.47	0.95
1:2:180:MSE:HE2	1:2:184:LEU:HG	1.50	0.94
1:1:391:LEU:HD22	1:1:416:ILE:HD12	1.52	0.90
1:1:484:ARG:HH11	1:1:484:ARG:HB2	1.34	0.90
1:1:423:ASP:HB2	1:1:425:ASN:H	1.35	0.90
1:2:352:GLN:HE21	1:2:387:MSE:HE1	1.37	0.89
1:1:235:THR:HA	1:1:282:MSE:HE1	1.56	0.88
1:2:278:ASN:HD21	1:2:300:LYS:H	1.17	0.88
1:1:13:ILE:HB	1:1:119:SER:HB3	1.56	0.87
1:1:31:VAL:HB	1:1:45:ILE:HG22	1.56	0.87
1:1:400:TRP:HE3	1:1:407:LEU:HD12	1.39	0.87
1:1:8:ILE:H	1:1:8:ILE:HD12	1.41	0.85
1:1:278:ASN:HD21	1:1:300:LYS:H	1.21	0.85
1:2:281:MSE:HE2	1:2:338:ILE:HG12	1.58	0.84
1:1:168:THR:HG22	1:1:170:ILE:H	1.42	0.83
1:1:400:TRP:CE3	1:1:407:LEU:HD12	2.13	0.82
1:2:340:GLY:O	1:2:363:THR:HB	1.77	0.82
1:1:329:ALA:HA	1:1:332:GLN:HE21	1.45	0.81
1:1:329:ALA:HA	1:1:332:GLN:NE2	1.96	0.80
1:2:10:ARG:HA	1:2:13:ILE:HG23	1.64	0.80
1:1:120:ARG:NH1	1:1:120:ARG:HB3	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:257:ILE:HD11	1:2:283:PHE:C	2.09	0.78
1:1:236:PRO:HD3	1:1:282:MSE:HE3	1.66	0.78
1:2:369:ILE:N	1:2:369:ILE:HD12	1.99	0.78
1:2:156:ILE:O	1:2:168:THR:HB	1.84	0.77
1:2:501:GLU:H	1:2:501:GLU:CD	1.93	0.77
1:2:281:MSE:HE3	1:2:284:ILE:HD11	1.66	0.76
1:1:120:ARG:HB3	1:1:120:ARG:HH11	1.48	0.76
1:1:295:ASP:O	1:2:331:ARG:NH2	2.19	0.76
1:2:321:ASP:OD1	1:2:323:TYR:HB3	1.86	0.75
1:1:185:THR:HG21	1:1:192:ILE:H	1.51	0.75
1:1:235:THR:HG21	1:1:489:VAL:HG21	1.69	0.75
1:2:35:TRP:CD2	1:2:38:GLU:HB3	2.23	0.74
1:2:473:ARG:HH11	1:2:504:MSE:HE1	1.51	0.74
1:1:377:GLU:OE1	1:1:385:ARG:HD2	1.88	0.73
1:2:146:ASP:OD2	1:2:406:ARG:NH2	2.22	0.73
1:2:12:HIS:CD2	1:2:99:VAL:HG21	2.23	0.73
1:1:13:ILE:HB	1:1:119:SER:CB	2.19	0.73
1:1:278:ASN:ND2	1:1:299:ILE:HA	2.04	0.73
1:1:475:LEU:HD23	1:1:478:MSE:HE3	1.69	0.73
1:1:231:ILE:O	1:1:232:GLU:HB2	1.87	0.72
1:1:380:PRO:HG3	1:2:384:PRO:HG3	1.71	0.72
1:2:424:LYS:H	1:2:424:LYS:HE2	1.55	0.71
1:1:9:LEU:HG	1:1:10:ARG:H	1.56	0.71
1:2:269:THR:HG22	1:2:365:HIS:CE1	2.26	0.71
1:2:236:PRO:O	1:2:240:ILE:HG13	1.90	0.70
1:1:492:TYR:CD2	1:1:507:MSE:HE1	2.26	0.70
1:2:253:LEU:O	1:2:257:ILE:HG23	1.90	0.70
1:2:13:ILE:HG13	1:2:14:ARG:H	1.57	0.70
1:1:379:GLU:HG3	1:1:380:PRO:HA	1.72	0.70
1:1:36:ILE:HD11	1:1:43:ALA:HB2	1.74	0.70
1:2:25:GLY:O	1:2:28:SER:HB3	1.92	0.69
1:2:203:LEU:HB3	1:2:204:PRO:HD2	1.73	0.69
1:1:419:ILE:HG23	1:1:425:ASN:OD1	1.93	0.69
1:1:51:GLU:O	1:1:53:ARG:HG2	1.93	0.69
1:1:246:PRO:HD3	1:1:441:HIS:CD2	2.28	0.69
1:1:8:ILE:HD12	1:1:8:ILE:N	2.07	0.68
1:2:352:GLN:HE21	1:2:387:MSE:CE	2.07	0.68
1:1:180:MSE:HE3	1:1:183:ARG:HB3	1.75	0.67
1:1:398:THR:HG22	1:1:399:MSE:N	2.09	0.67
1:2:132:TYR:CD2	1:2:139:MSE:HG2	2.29	0.67
1:2:185:THR:HG21	1:2:192:ILE:HB	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:281:MSE:HE1	1:2:361:TYR:CD1	2.29	0.67
1:1:180:MSE:HE2	1:1:184:LEU:CG	2.23	0.66
1:2:10:ARG:HH12	1:2:37:GLN:HG3	1.60	0.66
1:1:292:SER:C	1:1:293:ILE:HD12	2.19	0.66
1:2:11:ARG:HG2	1:2:11:ARG:HH11	1.58	0.66
1:2:180:MSE:HA	1:2:180:MSE:HE3	1.76	0.66
1:2:350:LEU:HD13	1:2:354:MSE:HE3	1.77	0.66
1:1:219:PRO:HG3	1:2:297:ARG:HD3	1.77	0.66
1:1:355:SER:HA	1:1:390:PHE:CD2	2.31	0.65
1:2:57:TYR:HA	1:2:169:ASN:ND2	2.11	0.65
1:1:277:LEU:HD22	1:1:281:MSE:HG2	1.79	0.65
1:1:235:THR:HA	1:1:282:MSE:CE	2.26	0.65
1:1:330:LEU:HD12	1:1:353:ALA:HB2	1.77	0.65
1:1:44:ILE:HD11	1:1:59:LEU:HD22	1.78	0.65
1:1:409:ARG:HG2	1:1:409:ARG:HH11	1.61	0.65
1:2:108:GLU:C	1:2:110:ALA:H	2.04	0.65
1:1:384:PRO:HG2	1:1:387:MSE:CG	2.27	0.65
1:2:369:ILE:HD11	1:2:412:GLU:OE2	1.97	0.65
1:2:274:THR:OG1	2:2:513:PO4:P	2.55	0.64
1:1:139:MSE:HA	1:1:228:LYS:HE2	1.79	0.64
1:1:8:ILE:H	1:1:8:ILE:CD1	2.08	0.64
1:1:134:LEU:HD22	1:1:134:LEU:H	1.63	0.64
1:1:52:PHE:HD1	1:1:52:PHE:H	1.46	0.64
1:1:45:ILE:HG12	1:1:163:TYR:CE1	2.33	0.64
1:2:278:ASN:ND2	1:2:299:ILE:HA	2.12	0.64
1:1:409:ARG:HD2	1:1:434:TRP:CE2	2.34	0.63
1:1:398:THR:HG22	1:1:399:MSE:H	1.62	0.63
1:2:233:PRO:HG2	1:2:300:LYS:HB3	1.81	0.63
1:1:32:GLU:HG2	1:1:33:GLU:N	2.14	0.63
1:1:258:GLU:OE2	1:1:471:ARG:NH2	2.31	0.63
1:1:484:ARG:HH11	1:1:484:ARG:CB	2.10	0.63
1:2:118:TYR:C	1:2:120:ARG:H	2.06	0.63
1:2:219:PRO:O	1:2:220:ARG:HB2	1.98	0.63
1:1:401:VAL:HA	1:1:405:THR:O	1.99	0.62
1:1:492:TYR:O	1:1:495:ALA:HB3	1.98	0.62
1:2:473:ARG:HD3	1:2:504:MSE:HE1	1.80	0.62
1:1:12:HIS:HD2	1:1:99:VAL:HG21	1.64	0.62
1:1:342:VAL:HG23	1:1:342:VAL:O	1.98	0.62
1:2:415:GLU:OE1	1:2:449:LYS:HB2	1.98	0.62
1:1:134:LEU:H	1:1:134:LEU:CD2	2.12	0.62
1:1:5:HIS:CD2	1:1:130:PHE:HB2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:8:ILE:O	1:1:11:ARG:HD3	1.98	0.62
1:1:35:TRP:CZ3	1:1:39:PRO:HA	2.35	0.62
1:2:297:ARG:NH2	1:2:299:ILE:O	2.32	0.61
1:2:420:ASP:O	1:2:424:LYS:HA	2.00	0.61
1:2:168:THR:HG23	1:2:170:ILE:H	1.65	0.61
1:2:473:ARG:HH11	1:2:504:MSE:CE	2.13	0.61
1:2:6:TYR:CD2	1:2:37:GLN:HG2	2.35	0.61
1:2:271:SER:N	2:2:514:PO4:O1	2.33	0.61
1:1:488:GLU:OE1	1:1:488:GLU:HA	1.99	0.61
1:2:190:LYS:HD2	1:2:201:ALA:HB2	1.83	0.61
1:1:81:ILE:HB	1:1:84:LEU:HD12	1.81	0.61
1:1:238:ASP:O	1:1:242:LYS:HG2	2.00	0.61
1:1:235:THR:HG22	1:1:238:ASP:H	1.66	0.61
1:2:295:ASP:HA	1:2:311:THR:HB	1.82	0.61
1:1:384:PRO:HG2	1:1:387:MSE:HG2	1.83	0.61
1:2:180:MSE:HE1	1:2:183:ARG:HD2	1.83	0.61
1:2:212:THR:HG22	1:2:223:SER:H	1.66	0.60
1:2:313:THR:O	1:2:313:THR:HG23	2.00	0.60
1:1:32:GLU:HG2	1:1:33:GLU:H	1.66	0.60
1:1:85:GLN:HE21	1:1:85:GLN:HA	1.66	0.60
1:2:234:LEU:HD12	1:2:275:THR:HG21	1.83	0.60
1:1:119:SER:C	1:1:121:MSE:H	2.08	0.60
1:1:217:VAL:HG13	1:2:310:VAL:O	2.01	0.60
1:1:413:VAL:HG23	1:1:432:VAL:HB	1.83	0.60
1:2:8:ILE:HD13	1:2:92:GLU:HA	1.82	0.60
1:1:235:THR:O	1:1:238:ASP:HB2	2.02	0.60
1:2:498:ARG:HG3	1:2:498:ARG:HH11	1.65	0.60
1:2:70:VAL:O	1:2:73:ALA:HB3	2.02	0.60
1:1:442:ILE:HD12	1:1:442:ILE:N	2.16	0.60
1:2:502:LEU:O	1:2:506:LYS:HG3	2.02	0.59
1:2:281:MSE:HE2	1:2:338:ILE:CG1	2.31	0.59
1:2:10:ARG:HA	1:2:13:ILE:CG2	2.31	0.59
1:2:180:MSE:CE	1:2:183:ARG:HD2	2.33	0.59
1:2:409:ARG:HD2	1:2:434:TRP:CE2	2.38	0.59
1:2:501:GLU:CD	1:2:501:GLU:N	2.60	0.59
1:1:171:VAL:O	1:1:172:LEU:HD23	2.02	0.59
1:1:326:LEU:HD13	1:1:349:THR:HB	1.85	0.59
1:2:450:LEU:HD11	1:2:468:MSE:CE	2.32	0.59
1:1:51:GLU:O	1:1:53:ARG:N	2.36	0.59
1:2:23:GLU:CD	1:2:23:GLU:H	2.10	0.59
1:1:489:VAL:O	1:1:493:ILE:HG13	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:474:TYR:CD2	1:1:478:MSE:HE2	2.38	0.58
1:2:144:VAL:O	1:2:228:LYS:HE2	2.02	0.58
1:1:215:THR:CG2	1:1:221:GLY:HA2	2.27	0.58
1:1:344:GLY:HA2	1:1:381:LEU:HD12	1.83	0.58
1:2:369:ILE:N	1:2:369:ILE:CD1	2.65	0.58
1:2:416:ILE:N	1:2:416:ILE:HD12	2.19	0.58
1:1:168:THR:HG22	1:1:170:ILE:N	2.13	0.58
1:2:10:ARG:O	1:2:13:ILE:HG12	2.04	0.58
1:2:168:THR:CG2	1:2:170:ILE:H	2.16	0.58
1:1:323:TYR:CE1	1:1:327:ARG:NE	2.71	0.58
1:2:12:HIS:O	1:2:13:ILE:C	2.47	0.58
1:1:12:HIS:CD2	1:1:99:VAL:HG21	2.39	0.58
1:2:215:THR:HA	1:2:218:THR:O	2.03	0.58
1:2:58:ALA:N	1:2:169:ASN:HD21	2.02	0.58
1:1:198:ILE:HD12	1:2:320:ILE:HD13	1.86	0.57
1:1:278:ASN:HD21	1:1:300:LYS:N	1.97	0.57
1:1:175:GLU:HG3	1:1:176:LYS:N	2.19	0.57
1:1:197:PRO:O	1:1:212:THR:HA	2.04	0.57
1:1:364:LEU:HD23	1:1:365:HIS:N	2.19	0.57
1:2:270:ALA:N	2:2:512:PO4:O1	2.37	0.57
1:2:446:MSE:HG2	1:2:447:PRO:CD	2.27	0.57
1:1:492:TYR:HD2	1:1:507:MSE:CE	2.18	0.57
1:2:118:TYR:O	1:2:120:ARG:N	2.33	0.57
1:2:136:ASP:HB3	1:2:137:PRO:HD3	1.86	0.57
1:1:156:ILE:O	1:1:168:THR:HB	2.05	0.57
1:1:19:LEU:H	1:1:120:ARG:HD3	1.69	0.57
1:1:295:ASP:CG	1:1:343:ARG:HH22	2.12	0.57
1:1:475:LEU:HD23	1:1:478:MSE:CE	2.35	0.57
1:2:272:GLY:N	2:2:514:PO4:O1	2.38	0.57
1:2:446:MSE:HE3	1:2:450:LEU:HD22	1.87	0.57
1:1:423:ASP:HB2	1:1:425:ASN:N	2.14	0.56
1:1:434:TRP:CZ3	1:1:436:PRO:HB3	2.40	0.56
1:2:173:ASP:CG	1:2:176:LYS:HD3	2.30	0.56
1:1:263:ALA:HA	1:1:393:ILE:O	2.05	0.56
1:2:485:ASN:N	1:2:485:ASN:HD22	2.02	0.56
1:1:350:LEU:HD11	1:1:360:SER:HB3	1.88	0.56
1:2:116:ASN:ND2	1:2:120:ARG:HH21	2.03	0.56
1:1:291:VAL:HG11	1:1:329:ALA:HB1	1.87	0.56
1:1:33:GLU:HG2	1:1:42:LYS:HE2	1.88	0.56
1:1:203:LEU:HD21	1:1:209:LEU:HD22	1.87	0.56
1:1:219:PRO:C	1:1:221:GLY:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:314:GLY:O	1:2:319:GLU:HG3	2.04	0.56
1:1:198:ILE:HD13	1:2:325:LEU:HD21	1.86	0.55
1:1:301:LEU:HB2	1:1:306:TRP:CZ3	2.41	0.55
1:1:139:MSE:SE	1:1:228:LYS:HD3	2.56	0.55
1:2:478:MSE:HE1	1:2:489:VAL:HG13	1.87	0.55
1:1:492:TYR:CD2	1:1:507:MSE:CE	2.89	0.55
1:2:252:TYR:HA	1:2:468:MSE:HE2	1.88	0.55
1:2:450:LEU:HD11	1:2:468:MSE:HE3	1.86	0.55
1:1:245:VAL:HG22	1:1:410:THR:OG1	2.07	0.55
1:2:24:PHE:HB3	1:2:28:SER:OG	2.07	0.55
1:1:11:ARG:N	1:1:13:ILE:HD12	2.21	0.55
1:1:215:THR:HG22	1:1:221:GLY:CA	2.27	0.55
1:2:180:MSE:HE2	1:2:184:LEU:CG	2.31	0.55
1:2:465:TYR:HE1	1:2:469:LEU:HD11	1.72	0.55
1:1:344:GLY:CA	1:1:381:LEU:HD12	2.37	0.55
1:1:364:LEU:HD13	1:1:372:MSE:HG3	1.87	0.55
1:1:330:LEU:HD23	1:1:330:LEU:O	2.07	0.54
1:2:255:LEU:HD23	1:2:471:ARG:CZ	2.38	0.54
1:2:379:GLU:HG3	1:2:380:PRO:HA	1.87	0.54
1:2:433:LYS:NZ	1:2:433:LYS:HB3	2.22	0.54
1:1:273:LYS:HD2	1:1:363:THR:HG23	1.89	0.54
1:1:391:LEU:HD23	1:1:392:ASP:N	2.23	0.54
1:2:121:MSE:HG2	1:2:125:LEU:CD2	2.38	0.54
1:1:144:VAL:O	1:1:144:VAL:HG23	2.06	0.54
1:2:465:TYR:CE1	1:2:469:LEU:HD11	2.41	0.54
1:1:473:ARG:HD3	1:1:504:MSE:HE1	1.89	0.54
1:2:144:VAL:HG13	1:2:158:ILE:HB	1.89	0.54
1:2:160:HIS:ND1	1:2:163:TYR:HD1	2.05	0.54
1:1:293:ILE:HD12	1:1:293:ILE:N	2.23	0.54
1:1:397:GLN:NE2	1:1:410:THR:HA	2.23	0.54
1:2:478:MSE:HG2	1:2:507:MSE:CE	2.38	0.54
1:2:84:LEU:HA	1:2:94:ARG:HB2	1.90	0.53
1:2:342:VAL:CG2	1:2:364:LEU:HD23	2.38	0.53
1:1:219:PRO:HD2	1:2:308:ALA:O	2.08	0.53
1:1:304:GLU:O	1:1:306:TRP:N	2.41	0.53
1:1:369:ILE:O	1:1:373:VAL:HG23	2.08	0.53
1:2:14:ARG:HH11	1:2:14:ARG:HB2	1.73	0.53
1:1:146:ASP:OD2	1:2:333:ARG:HD3	2.09	0.53
1:1:389:GLN:HB3	1:1:419:ILE:HG13	1.90	0.53
1:2:300:LYS:HB2	1:2:300:LYS:NZ	2.23	0.53
1:1:84:LEU:HD13	1:1:129:PHE:CE2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:420:ASP:O	1:1:423:ASP:OD2	2.26	0.53
1:2:108:GLU:C	1:2:110:ALA:N	2.67	0.53
1:2:8:ILE:O	1:2:11:ARG:HB2	2.08	0.52
1:2:116:ASN:HD22	1:2:120:ARG:HH21	1.56	0.52
1:1:37:GLN:CG	1:1:140:GLU:HG2	2.39	0.52
1:1:40:PHE:N	1:1:40:PHE:CD1	2.77	0.52
1:2:121:MSE:HG2	1:2:125:LEU:HD23	1.92	0.52
1:2:446:MSE:CG	1:2:447:PRO:HD2	2.27	0.52
1:2:212:THR:HG22	1:2:223:SER:N	2.24	0.52
1:2:423:ASP:HB2	1:2:425:ASN:HD21	1.75	0.52
1:2:326:LEU:HD13	1:2:349:THR:CG2	2.39	0.52
1:2:257:ILE:HD11	1:2:284:ILE:N	2.24	0.52
1:1:138:LEU:O	1:1:144:VAL:HG21	2.10	0.52
1:1:198:ILE:CD1	1:2:320:ILE:HD13	2.39	0.52
1:2:14:ARG:NH1	1:2:118:TYR:CE1	2.78	0.52
1:2:274:THR:OG1	2:2:513:PO4:O3	2.27	0.52
1:1:237:ILE:HG22	1:1:484:ARG:HD2	1.92	0.51
1:2:35:TRP:CE3	1:2:38:GLU:HB3	2.45	0.51
1:1:29:ARG:O	1:1:46:VAL:HG13	2.10	0.51
1:1:322:MSE:HE1	1:1:341:GLU:O	2.10	0.51
1:1:409:ARG:HG2	1:1:409:ARG:NH1	2.21	0.51
1:2:155:PRO:HA	1:2:171:VAL:HG22	1.93	0.51
1:2:233:PRO:CG	1:2:300:LYS:HB3	2.40	0.51
1:2:239:LEU:HD22	1:2:244:THR:HG21	1.92	0.51
1:2:502:LEU:O	1:2:502:LEU:HD22	2.10	0.51
1:2:35:TRP:HA	1:2:42:LYS:HG3	1.93	0.51
1:1:403:GLY:C	1:1:405:THR:H	2.17	0.51
1:2:10:ARG:CA	1:2:13:ILE:HG23	2.38	0.51
1:1:189:GLY:O	1:1:190:LYS:HD3	2.11	0.51
1:1:343:ARG:HB3	1:2:352:GLN:HE22	1.76	0.51
1:1:57:TYR:HE2	1:1:59:LEU:HD12	1.75	0.51
1:2:342:VAL:O	1:2:342:VAL:HG23	2.11	0.51
1:2:60:GLU:HB3	1:2:61:PRO:HD2	1.92	0.51
1:2:194:ILE:HG23	1:2:216:GLU:HG2	1.92	0.51
1:1:487:LYS:O	1:1:491:ARG:HG3	2.11	0.51
1:2:447:PRO:HG2	1:2:450:LEU:HD22	1.92	0.51
1:1:402:ARG:HA	1:1:402:ARG:NE	2.26	0.50
1:1:413:VAL:CG2	1:1:432:VAL:HB	2.40	0.50
1:1:44:ILE:N	1:1:44:ILE:HD12	2.26	0.50
1:1:132:TYR:C	1:1:183:ARG:HH12	2.19	0.50
1:1:277:LEU:HD22	1:1:281:MSE:CG	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:349:THR:O	1:1:352:GLN:HB2	2.11	0.50
1:1:421:PRO:O	1:1:422:VAL:O	2.30	0.50
1:1:122:LEU:HD22	1:1:126:PHE:HE1	1.76	0.50
1:1:430:GLN:O	1:1:444:VAL:HG23	2.12	0.50
1:1:488:GLU:OE1	1:1:491:ARG:NH1	2.44	0.50
1:2:393:ILE:HG22	1:2:395:LEU:HD12	1.93	0.50
1:1:266:VAL:HG12	1:1:366:ALA:O	2.11	0.50
1:1:398:THR:OG1	1:1:411:LYS:HB2	2.12	0.50
1:2:11:ARG:HG2	1:2:11:ARG:NH1	2.25	0.50
1:1:173:ASP:OD2	1:1:176:LYS:HB2	2.11	0.50
1:1:236:PRO:HD3	1:1:282:MSE:CE	2.39	0.50
1:2:13:ILE:HG13	1:2:14:ARG:N	2.24	0.50
1:1:52:PHE:CD1	1:1:52:PHE:N	2.78	0.50
1:2:118:TYR:C	1:2:120:ARG:N	2.67	0.50
1:2:219:PRO:O	1:2:220:ARG:CB	2.59	0.50
1:1:12:HIS:O	1:1:118:TYR:HE2	1.95	0.50
1:1:134:LEU:HD22	1:1:134:LEU:N	2.27	0.50
1:1:122:LEU:HD22	1:1:126:PHE:CE1	2.47	0.49
1:2:23:GLU:O	1:2:23:GLU:HG2	2.11	0.49
1:1:339:VAL:O	1:1:340:GLY:C	2.55	0.49
1:2:197:PRO:O	1:2:212:THR:HA	2.11	0.49
1:1:138:LEU:O	1:1:144:VAL:CG2	2.60	0.49
1:1:192:ILE:HD11	1:1:213:PHE:N	2.27	0.49
1:1:79:LYS:C	1:1:81:ILE:H	2.20	0.49
1:1:329:ALA:O	1:1:332:GLN:HG2	2.12	0.49
1:2:9:LEU:C	1:2:9:LEU:HD23	2.38	0.49
1:2:18:LEU:HB3	1:2:120:ARG:HD3	1.95	0.49
1:1:434:TRP:CH2	1:1:436:PRO:HB3	2.48	0.49
1:2:14:ARG:HD3	1:2:115:ASP:HA	1.95	0.49
1:2:498:ARG:HH11	1:2:498:ARG:CG	2.26	0.49
1:2:162:LYS:HD2	1:2:163:TYR:CE1	2.47	0.49
1:1:60:GLU:HB3	1:1:61:PRO:HD2	1.95	0.49
1:1:356:THR:O	1:1:356:THR:HG22	2.13	0.49
1:2:15:SER:HB3	1:2:119:SER:OG	2.12	0.49
1:2:20:GLU:HG3	1:2:62:THR:OG1	2.12	0.49
1:2:86:ASP:OD1	1:2:89:VAL:HG23	2.13	0.49
1:1:143:ASN:HB3	1:1:160:HIS:CE1	2.48	0.49
1:2:173:ASP:OD2	1:2:176:LYS:HD3	2.13	0.49
1:2:273:LYS:HE2	1:2:363:THR:CG2	2.43	0.49
1:1:6:TYR:O	1:1:10:ARG:HB3	2.13	0.48
1:1:155:PRO:HA	1:1:171:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:204:PRO:C	1:1:206:GLY:H	2.21	0.48
1:2:281:MSE:HG2	1:2:338:ILE:HD13	1.95	0.48
1:1:48:ASN:O	1:1:49:GLU:C	2.56	0.48
1:2:465:TYR:O	1:2:468:MSE:HB3	2.13	0.48
1:1:22:PRO:HB3	1:1:24:PHE:CZ	2.48	0.48
1:1:85:GLN:HA	1:1:85:GLN:NE2	2.28	0.48
1:2:494:HIS:O	1:2:497:TYR:HB2	2.13	0.48
1:1:229:PHE:CE1	1:1:300:LYS:HE3	2.48	0.48
1:1:417:LEU:HD21	1:1:448:LYS:HD3	1.96	0.48
1:1:229:PHE:O	1:1:231:ILE:HG13	2.14	0.48
1:1:441:HIS:C	1:1:442:ILE:HD12	2.38	0.48
2:2:512:PO4:O4	2:2:514:PO4:O3	2.32	0.48
1:1:126:PHE:HA	1:1:130:PHE:CD1	2.48	0.48
1:2:424:LYS:HE2	1:2:424:LYS:N	2.24	0.48
1:1:225:THR:C	1:1:226:ILE:HG13	2.38	0.48
1:1:376:LEU:HA	1:1:381:LEU:HD23	1.96	0.48
1:1:278:ASN:HD21	1:1:299:ILE:HA	1.78	0.48
1:1:279:ALA:HA	1:1:282:MSE:CE	2.44	0.48
1:2:254:TRP:CE3	1:2:471:ARG:HB3	2.49	0.47
1:2:398:THR:CG2	1:2:411:LYS:HB2	2.44	0.47
1:1:272:GLY:O	1:1:273:LYS:C	2.57	0.47
1:1:356:THR:O	1:1:356:THR:CG2	2.61	0.47
1:2:67:GLU:HB3	1:2:117:PHE:HE1	1.79	0.47
1:2:451:GLU:HG2	1:2:461:VAL:HG21	1.94	0.47
1:1:356:THR:CG2	1:1:358:HIS:CE1	2.98	0.47
1:2:61:PRO:HB2	1:2:120:ARG:HG3	1.97	0.47
1:2:384:PRO:HG2	1:2:387:MSE:CG	2.44	0.47
1:2:431:PHE:CD1	1:2:432:VAL:HG23	2.49	0.47
1:2:489:VAL:O	1:2:493:ILE:HG13	2.14	0.47
1:1:9:LEU:HD11	1:1:122:LEU:HB3	1.96	0.47
1:1:168:THR:CG2	1:1:169:ASN:N	2.78	0.47
1:1:384:PRO:HG2	1:1:387:MSE:HG3	1.96	0.47
1:2:498:ARG:HA	1:2:498:ARG:HD3	1.76	0.47
1:1:120:ARG:NH1	1:1:120:ARG:CB	2.74	0.47
1:2:6:TYR:CG	1:2:37:GLN:HG2	2.50	0.47
1:2:14:ARG:HD2	1:2:118:TYR:CD1	2.50	0.47
1:2:18:LEU:HD13	1:2:119:SER:O	2.14	0.47
1:2:209:LEU:HD23	1:2:210:GLN:H	1.80	0.47
1:2:341:GLU:HA	1:2:363:THR:O	2.14	0.47
1:2:473:ARG:HG2	1:2:504:MSE:HE1	1.96	0.47
1:1:460:SER:OG	1:1:463:GLU:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:14:ARG:O	1:2:15:SER:HB2	2.15	0.47
1:2:45:ILE:N	1:2:45:ILE:HD12	2.30	0.47
1:1:68:ALA:O	1:1:71:ILE:HG22	2.15	0.47
1:1:203:LEU:HB3	1:1:204:PRO:HD2	1.95	0.47
1:2:96:GLU:C	1:2:98:LEU:N	2.69	0.47
1:2:241:GLU:CD	1:2:484:ARG:HE	2.23	0.47
1:2:423:ASP:O	1:2:424:LYS:C	2.58	0.47
1:1:185:THR:HG22	1:1:190:LYS:O	2.14	0.47
1:2:298:GLU:OE1	2:2:513:PO4:O3	2.33	0.47
1:2:188:SER:OG	1:2:203:LEU:HD23	2.15	0.46
1:2:263:ALA:HB2	1:2:393:ILE:HB	1.97	0.46
1:2:406:ARG:O	1:2:407:LEU:HD13	2.15	0.46
1:1:188:SER:HB3	1:1:203:LEU:HD23	1.97	0.46
1:1:198:ILE:HD13	1:2:325:LEU:CD2	2.46	0.46
1:1:232:GLU:OE1	1:1:232:GLU:HA	2.14	0.46
1:1:235:THR:H	1:1:238:ASP:HB2	1.81	0.46
1:1:386:SER:HA	1:1:419:ILE:CD1	2.45	0.46
1:2:19:LEU:HD12	1:2:35:TRP:CZ3	2.50	0.46
1:2:244:THR:HG23	1:2:245:VAL:HG23	1.96	0.46
1:2:352:GLN:HG2	1:2:387:MSE:CE	2.45	0.46
1:2:473:ARG:CD	1:2:504:MSE:HE1	2.44	0.46
1:1:125:LEU:O	1:1:129:PHE:HD1	1.99	0.46
1:2:159:TYR:CE1	1:2:164:GLY:HA2	2.50	0.46
1:1:7:ASP:O	1:1:9:LEU:O	2.33	0.46
1:1:419:ILE:CG2	1:1:420:ASP:N	2.79	0.46
1:2:232:GLU:HA	1:2:233:PRO:HD3	1.75	0.46
1:1:244:THR:HG22	1:1:245:VAL:HG23	1.98	0.46
1:1:330:LEU:CD1	1:1:353:ALA:HB2	2.45	0.46
1:2:149:CYS:O	1:2:223:SER:HB2	2.16	0.46
1:1:279:ALA:HA	1:1:282:MSE:HE3	1.97	0.46
1:2:209:LEU:CD2	1:2:210:GLN:N	2.78	0.46
1:2:278:ASN:HD21	1:2:300:LYS:N	1.99	0.46
1:1:5:HIS:HA	1:1:91:LEU:HD21	1.98	0.46
1:1:37:GLN:HG2	1:1:140:GLU:HG2	1.98	0.46
1:1:136:ASP:N	1:1:137:PRO:CD	2.79	0.46
1:2:269:THR:O	1:2:270:ALA:HB3	2.15	0.46
1:1:39:PRO:HD2	1:1:40:PHE:CE1	2.50	0.46
1:2:23:GLU:CD	1:2:23:GLU:N	2.75	0.46
1:1:369:ILE:HD11	1:1:414:ASN:CB	2.47	0.45
1:2:381:LEU:HD12	1:2:381:LEU:N	2.30	0.45
1:2:384:PRO:HG2	1:2:387:MSE:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:ASP:O	1:1:11:ARG:HD2	2.17	0.45
1:1:272:GLY:N	2:1:512:PO4:O4	2.49	0.45
1:2:9:LEU:HD11	1:2:123:TYR:HA	1.98	0.45
1:1:235:THR:CG2	1:1:237:ILE:HB	2.46	0.45
1:1:511:LEU:C	1:1:511:LEU:HD23	2.41	0.45
1:2:423:ASP:HB2	1:2:425:ASN:ND2	2.32	0.45
1:1:9:LEU:HG	1:1:10:ARG:N	2.25	0.45
1:1:271:SER:O	1:1:408:ARG:HG2	2.16	0.45
1:1:314:GLY:O	1:1:315:MSE:C	2.60	0.45
1:2:401:VAL:O	1:2:401:VAL:HG23	2.16	0.45
1:2:99:VAL:HG13	1:2:118:TYR:OH	2.16	0.45
1:2:287:ASP:CG	1:2:498:ARG:HH21	2.24	0.45
1:1:356:THR:HG21	1:1:358:HIS:HE1	1.81	0.45
1:2:218:THR:O	1:2:218:THR:HG22	2.15	0.45
1:2:438:GLU:HB2	1:2:440:LYS:HG3	1.99	0.45
1:2:84:LEU:HD12	1:2:85:GLN:N	2.31	0.45
1:1:144:VAL:O	1:1:144:VAL:CG2	2.64	0.45
1:1:57:TYR:CE2	1:1:59:LEU:HD12	2.52	0.45
1:1:198:ILE:CD1	1:2:325:LEU:HD21	2.47	0.45
1:1:146:ASP:HB2	1:1:159:TYR:HB3	1.98	0.44
1:2:364:LEU:HD13	1:2:365:HIS:N	2.32	0.44
1:2:420:ASP:HA	1:2:421:PRO:HD3	1.81	0.44
1:1:241:GLU:HG3	1:1:479:LEU:HD21	1.99	0.44
1:2:504:MSE:O	1:2:508:GLU:HG2	2.16	0.44
1:2:89:VAL:HG12	1:2:90:ASP:N	2.33	0.44
1:2:139:MSE:HE1	1:2:226:ILE:HG21	2.00	0.44
1:2:395:LEU:HD12	1:2:395:LEU:N	2.33	0.44
1:1:234:LEU:HD12	1:1:234:LEU:HA	1.81	0.44
1:2:34:TYR:O	1:2:34:TYR:CD1	2.71	0.44
1:2:143:ASN:N	1:2:143:ASN:HD22	2.14	0.44
1:2:288:ALA:O	1:2:303:HIS:HE1	2.00	0.44
1:2:400:TRP:HB3	1:2:407:LEU:HB2	2.00	0.44
1:1:397:GLN:NE2	1:1:410:THR:CA	2.80	0.44
1:1:478:MSE:HG2	1:1:507:MSE:CE	2.47	0.44
1:2:302:TYR:HB3	1:2:490:THR:HG21	1.98	0.44
1:1:119:SER:O	1:1:121:MSE:N	2.49	0.44
1:2:277:LEU:O	1:2:281:MSE:HB2	2.18	0.44
1:1:342:VAL:O	1:1:342:VAL:CG2	2.65	0.44
1:2:342:VAL:HG23	1:2:364:LEU:HD23	2.00	0.44
1:1:506:LYS:HB3	1:1:511:LEU:OXT	2.18	0.44
1:2:9:LEU:C	1:2:11:ARG:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:118:TYR:O	1:1:121:MSE:HB3	2.18	0.43
1:1:235:THR:HG23	1:1:236:PRO:HD2	1.99	0.43
1:2:259:HIS:HE1	1:2:457:LEU:HD21	1.83	0.43
1:1:119:SER:C	1:1:121:MSE:N	2.76	0.43
1:1:262:SER:O	1:1:392:ASP:HB2	2.18	0.43
1:1:356:THR:HG22	1:1:358:HIS:CE1	2.52	0.43
1:1:364:LEU:HD23	1:1:364:LEU:C	2.43	0.43
1:1:65:SER:O	1:1:68:ALA:HB3	2.17	0.43
1:1:185:THR:HG21	1:1:192:ILE:HG22	2.00	0.43
1:1:237:ILE:HD12	1:1:237:ILE:N	2.33	0.43
1:2:287:ASP:OD1	1:2:498:ARG:NH2	2.51	0.43
1:1:260:LYS:HB3	1:1:359:ALA:HB2	2.00	0.43
1:1:330:LEU:HD23	1:1:330:LEU:C	2.42	0.43
1:2:61:PRO:HG2	1:2:124:TYR:CE1	2.54	0.43
1:2:64:SER:OG	1:2:67:GLU:HG3	2.18	0.43
1:2:114:THR:HB	1:2:117:PHE:H	1.84	0.43
1:2:239:LEU:O	1:2:244:THR:HG22	2.18	0.43
1:2:254:TRP:CD2	1:2:471:ARG:HD3	2.53	0.43
1:2:257:ILE:HD11	1:2:284:ILE:HA	1.99	0.43
1:1:391:LEU:HD23	1:1:391:LEU:C	2.44	0.43
1:1:492:TYR:HD2	1:1:507:MSE:HE2	1.83	0.43
1:2:485:ASN:N	1:2:485:ASN:ND2	2.65	0.43
1:1:126:PHE:HA	1:1:130:PHE:CE1	2.54	0.43
1:2:9:LEU:C	1:2:9:LEU:CD2	2.92	0.43
1:2:16:GLU:O	1:2:17:ASP:HB3	2.19	0.43
1:2:77:ASP:O	1:2:80:LYS:HB2	2.19	0.43
1:2:240:ILE:CG1	1:2:250:LEU:HD23	2.48	0.43
1:2:418:GLY:H	1:2:427:LEU:HB2	1.82	0.43
1:2:422:VAL:O	1:2:423:ASP:HB2	2.19	0.43
1:2:473:ARG:HD3	1:2:504:MSE:CE	2.45	0.43
1:1:218:THR:O	1:1:219:PRO:C	2.62	0.43
1:2:37:GLN:HE21	1:2:37:GLN:HB2	1.59	0.43
1:2:416:ILE:N	1:2:416:ILE:CD1	2.82	0.43
1:1:229:PHE:CE2	1:1:231:ILE:HD11	2.54	0.43
1:1:326:LEU:HD22	1:1:349:THR:HG22	2.00	0.43
1:2:57:TYR:CA	1:2:169:ASN:ND2	2.81	0.43
1:2:290:VAL:HB	1:2:306:TRP:HB2	2.01	0.43
1:2:173:ASP:OD2	1:2:173:ASP:C	2.61	0.43
1:2:485:ASN:HB2	1:2:488:GLU:HG2	2.01	0.43
1:1:240:ILE:HG21	1:1:479:LEU:HD12	2.00	0.42
1:1:442:ILE:N	1:1:442:ILE:CD1	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:9:LEU:O	1:2:11:ARG:N	2.51	0.42
1:2:235:THR:HG22	1:2:282:MSE:SE	2.69	0.42
1:2:302:TYR:CE1	1:2:487:LYS:HD3	2.54	0.42
1:1:160:HIS:HB3	1:1:163:TYR:HB2	2.01	0.42
1:1:277:LEU:CD2	1:1:281:MSE:HG2	2.48	0.42
1:1:415:GLU:HB2	1:1:429:ASN:O	2.19	0.42
1:1:235:THR:HG23	1:1:236:PRO:N	2.34	0.42
1:1:404:ASN:O	1:1:404:ASN:ND2	2.52	0.42
1:1:152:TYR:CD2	1:1:174:GLN:HA	2.54	0.42
1:1:419:ILE:HG22	1:1:420:ASP:N	2.33	0.42
1:2:194:ILE:HG23	1:2:216:GLU:CG	2.49	0.42
1:1:396:VAL:HB	1:1:412:GLU:HG2	2.02	0.42
1:2:152:TYR:CD2	1:2:174:GLN:HA	2.54	0.42
1:2:183:ARG:CB	1:2:183:ARG:HH11	2.33	0.42
1:2:430:GLN:O	1:2:444:VAL:CG2	2.67	0.42
1:1:35:TRP:CE3	1:1:38:GLU:HA	2.54	0.42
1:1:249:VAL:HG22	1:1:432:VAL:HG21	2.02	0.42
1:1:388:LEU:HB3	1:1:426:LEU:HD21	2.02	0.42
1:2:332:GLN:HB2	1:2:334:PRO:HD3	2.01	0.42
1:1:290:VAL:HG13	1:1:306:TRP:HB2	2.02	0.42
1:1:315:MSE:HE3	1:1:315:MSE:O	2.20	0.42
1:2:40:PHE:CD1	1:2:40:PHE:N	2.87	0.42
1:2:409:ARG:HG2	1:2:409:ARG:HH11	1.85	0.42
1:2:433:LYS:HB3	1:2:433:LYS:HZ3	1.84	0.42
1:1:53:ARG:HH21	1:1:167:GLU:HB2	1.85	0.42
1:1:284:ILE:HA	1:1:285:PRO:HD3	1.91	0.42
1:1:354:MSE:C	1:1:356:THR:N	2.76	0.42
1:2:340:GLY:O	1:2:341:GLU:HB2	2.20	0.42
1:2:350:LEU:HD13	1:2:354:MSE:CE	2.48	0.42
2:2:512:PO4:O4	2:2:514:PO4:O4	2.38	0.42
1:1:264:ILE:HD12	1:1:391:LEU:CD1	2.50	0.42
1:2:47:GLU:OE2	1:2:49:GLU:HB3	2.20	0.42
1:2:172:LEU:HA	1:2:176:LYS:HE2	2.02	0.42
1:2:262:SER:O	1:2:392:ASP:HB2	2.20	0.42
1:2:484:ARG:HG3	1:2:484:ARG:HH11	1.85	0.42
1:2:200:ASP:HB2	1:2:210:GLN:HE22	1.85	0.41
1:2:9:LEU:HD22	1:2:40:PHE:CZ	2.55	0.41
1:2:58:ALA:H	1:2:169:ASN:HD21	1.65	0.41
1:2:467:GLU:O	1:2:470:SER:HB3	2.20	0.41
1:2:484:ARG:HG3	1:2:484:ARG:NH1	2.34	0.41
1:1:26:SER:C	1:1:28:SER:H	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:208:ARG:NH2	1:2:331:ARG:NH1	2.68	0.41
1:1:235:THR:CG2	1:1:237:ILE:H	2.33	0.41
1:1:313:THR:HG23	1:1:315:MSE:H	1.84	0.41
1:2:145:GLU:OE2	1:2:406:ARG:NH1	2.54	0.41
1:2:257:ILE:HD11	1:2:283:PHE:O	2.20	0.41
1:2:492:TYR:CD2	1:2:507:MSE:HE1	2.55	0.41
1:2:398:THR:HG22	1:2:411:LYS:HB2	2.01	0.41
1:1:12:HIS:O	1:1:118:TYR:CE2	2.74	0.41
1:1:38:GLU:HA	1:1:39:PRO:HA	1.80	0.41
1:1:264:ILE:HD12	1:1:391:LEU:HD11	2.02	0.41
1:1:266:VAL:HG12	1:1:267:GLY:N	2.34	0.41
1:1:505:THR:O	1:1:509:GLU:HG2	2.21	0.41
1:2:23:GLU:N	1:2:23:GLU:OE2	2.54	0.41
1:2:326:LEU:HD13	1:2:349:THR:HG22	2.01	0.41
1:1:204:PRO:C	1:1:206:GLY:N	2.78	0.41
1:1:430:GLN:OE1	1:1:433:LYS:HE3	2.20	0.41
1:2:13:ILE:O	1:2:14:ARG:HB3	2.20	0.41
1:2:93:GLU:O	1:2:97:VAL:HG23	2.20	0.41
1:2:428:VAL:CG1	1:2:429:ASN:N	2.84	0.41
1:1:193:SER:O	1:1:196:ASN:C	2.63	0.41
1:2:53:ARG:HG2	1:2:53:ARG:HH11	1.84	0.41
1:2:209:LEU:HD22	1:2:210:GLN:N	2.36	0.41
1:2:363:THR:HG21	2:2:513:PO4:O1	2.21	0.41
1:2:492:TYR:O	1:2:495:ALA:HB3	2.21	0.41
1:1:57:TYR:HA	1:1:169:ASN:OD1	2.20	0.41
1:1:398:THR:HG22	1:1:399:MSE:O	2.20	0.41
1:1:409:ARG:HD2	1:1:434:TRP:CZ2	2.56	0.41
1:2:9:LEU:HD23	1:2:9:LEU:O	2.21	0.41
1:2:14:ARG:O	1:2:15:SER:CB	2.69	0.41
1:2:55:VAL:HG12	1:2:167:GLU:HB3	2.02	0.41
1:2:58:ALA:H	1:2:169:ASN:ND2	2.19	0.41
1:2:177:LEU:O	1:2:180:MSE:HB3	2.20	0.41
1:1:267:GLY:C	1:1:268:GLU:O	2.63	0.40
1:1:420:ASP:O	1:1:423:ASP:HB3	2.21	0.40
1:1:235:THR:HG22	1:1:237:ILE:N	2.37	0.40
1:1:386:SER:HA	1:1:419:ILE:HD13	2.04	0.40
1:2:70:VAL:O	1:2:74:LEU:HD23	2.21	0.40
1:2:168:THR:HG23	1:2:169:ASN:N	2.35	0.40
1:2:478:MSE:HG2	1:2:507:MSE:HE3	2.03	0.40
1:2:505:THR:O	1:2:509:GLU:HB2	2.21	0.40
1:1:35:TRP:CZ3	1:1:38:GLU:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:81:ILE:HG22	1:1:83:VAL:HG22	2.03	0.40
1:1:162:LYS:HE2	1:1:163:TYR:CZ	2.57	0.40
1:2:268:GLU:OE2	1:2:365:HIS:HE1	2.05	0.40
1:2:327:ARG:HB3	1:2:327:ARG:HH11	1.86	0.40
1:2:367:GLY:H	1:2:371:GLN:NE2	2.20	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	1	494/511 (97%)	417 (84%)	54 (11%)	23 (5%)	2	11
1	2	499/511 (98%)	441 (88%)	49 (10%)	9 (2%)	6	29
All	All	993/1022 (97%)	858 (86%)	103 (10%)	32 (3%)	3	17

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	11	ARG
1	1	52	PHE
1	1	68	ALA
1	2	13	ILE
1	1	120	ARG
1	1	329	ALA
1	1	405	THR
1	1	425	ASN
1	1	510	GLY
1	2	345	ARG
1	1	19	LEU
1	1	20	GLU
1	1	49	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	220	ARG
1	1	268	GLU
1	1	273	LYS
1	1	305	ASN
1	2	15	SER
1	2	104	LYS
1	2	119	SER
1	1	48	ASN
1	1	50	ASP
1	1	174	GLN
1	1	332	GLN
1	2	10	ARG
1	2	288	ALA
1	2	341	GLU
1	2	437	LYS
1	1	345	ARG
1	1	422	VAL
1	1	80	LYS
1	1	286	PRO

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	1	406/439 (92%)	372 (92%)	34 (8%)	10	33
1	2	444/439 (101%)	406 (91%)	38 (9%)	10	32
All	All	850/878 (97%)	778 (92%)	72 (8%)	10	33

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	ILE
1	1	13	ILE
1	1	39	PRO
1	1	40	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	47	GLU
1	1	50	ASP
1	1	51	GLU
1	1	59	LEU
1	1	134	LEU
1	1	174	GLN
1	1	228	LYS
1	1	234	LEU
1	1	235	THR
1	1	268	GLU
1	1	277	LEU
1	1	290	VAL
1	1	295	ASP
1	1	311	THR
1	1	326	LEU
1	1	332	GLN
1	1	385	ARG
1	1	397	GLN
1	1	406	ARG
1	1	409	ARG
1	1	424	LYS
1	1	425	ASN
1	1	426	LEU
1	1	450	LEU
1	1	479	LEU
1	1	484	ARG
1	1	487	LYS
1	1	488	GLU
1	1	501	GLU
1	1	504	MSE
1	2	11	ARG
1	2	14	ARG
1	2	18	LEU
1	2	20	GLU
1	2	37	GLN
1	2	40	PHE
1	2	84	LEU
1	2	168	THR
1	2	177	LEU
1	2	183	ARG
1	2	186	GLN
1	2	209	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	212	THR
1	2	216	GLU
1	2	232	GLU
1	2	245	VAL
1	2	250	LEU
1	2	257	ILE
1	2	265	VAL
1	2	268	GLU
1	2	269	THR
1	2	300	LYS
1	2	309	GLU
1	2	311	THR
1	2	319	GLU
1	2	326	LEU
1	2	350	LEU
1	2	363	THR
1	2	369	ILE
1	2	407	LEU
1	2	424	LYS
1	2	433	LYS
1	2	444	VAL
1	2	467	GLU
1	2	477	LEU
1	2	491	ARG
1	2	502	LEU
1	2	504	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	85	GLN
1	1	161	GLN
1	1	278	ASN
1	1	303	HIS
1	1	332	GLN
1	1	358	HIS
1	1	397	GLN
1	1	404	ASN
1	1	429	ASN
1	1	485	ASN
1	1	494	HIS
1	2	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	116	ASN
1	2	143	ASN
1	2	174	GLN
1	2	210	GLN
1	2	259	HIS
1	2	278	ASN
1	2	303	HIS
1	2	352	GLN
1	2	365	HIS
1	2	370	ASN
1	2	371	GLN
1	2	389	GLN
1	2	414	ASN
1	2	425	ASN
1	2	430	GLN
1	2	441	HIS
1	2	485	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	1	512	-	4,4,4	1.64	1 (25%)	6,6,6	0.81	0
2	PO4	2	512	-	4,4,4	1.78	1 (25%)	6,6,6	1.01	0
2	PO4	2	514	-	4,4,4	1.69	1 (25%)	6,6,6	1.04	0
2	PO4	2	513	-	4,4,4	1.42	1 (25%)	6,6,6	1.32	2 (33%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	512	PO4	P-O1	3.07	1.57	1.50
2	1	512	PO4	P-O1	2.76	1.57	1.50
2	2	514	PO4	P-O1	2.74	1.57	1.50
2	2	513	PO4	P-O1	2.23	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	513	PO4	O3-P-O2	2.17	114.65	107.91
2	2	513	PO4	O3-P-O1	-2.06	103.67	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	512	PO4	1	0
2	2	512	PO4	3	0
2	2	514	PO4	4	0
2	2	513	PO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	481/511 (94%)	-0.11	8 (1%) 69 48	24, 58, 118, 127	0
1	2	487/511 (95%)	-0.22	4 (0%) 82 66	32, 56, 89, 104	0
All	All	968/1022 (94%)	-0.16	12 (1%) 76 57	24, 57, 110, 127	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	296	THR	3.1
1	1	28	SER	2.9
1	2	119	SER	2.7
1	1	90	ASP	2.4
1	1	330	LEU	2.4
1	1	510	GLY	2.4
1	1	485	ASN	2.3
1	1	92	GLU	2.2
1	2	13	ILE	2.2
1	1	332	GLN	2.1
1	1	83	VAL	2.1
1	2	405	THR	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	2	513	5/5	0.68	0.25	53,53,55,57	5
2	PO4	1	512	5/5	0.75	0.18	51,52,53,54	5
2	PO4	2	512	5/5	0.83	0.20	55,57,57,57	5
2	PO4	2	514	5/5	0.89	0.10	61,61,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.