



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:29 PM UTC

PDB ID : 1WTH / pdb_00001wth
Title : Crystal structure of gp5-S351L mutant and gp27 complex
Authors : Kanamaru, S.; Ishiwata, Y.; Suzuki, T.; Rossmann, M.G.; Arisaka, F.
Deposited on : 2004-11-23
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

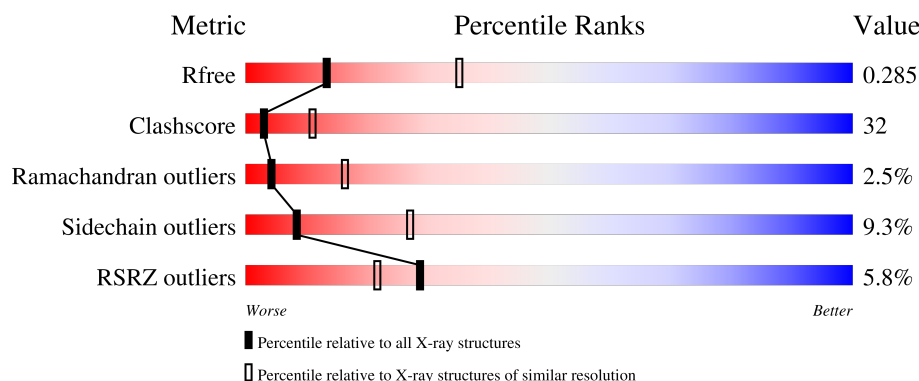
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	584	5% 55% 35% 7% ..
2	D	391	7% 43% 40% 8% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7575 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 Tail-associated lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4396	2727	777	870	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	LEU	SER	engineered mutation	UNP P16009
A	576	SER	-	expression tag	UNP P16009
A	577	VAL	-	expression tag	UNP P16009
A	578	ASP	-	expression tag	UNP P16009
A	579	HIS	-	expression tag	UNP P16009
A	580	HIS	-	expression tag	UNP P16009
A	581	HIS	-	expression tag	UNP P16009
A	582	HIS	-	expression tag	UNP P16009
A	583	HIS	-	expression tag	UNP P16009
A	584	HIS	-	expression tag	UNP P16009

- Molecule 2 is a protein called Baseplate structural protein Gp27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	361	Total	C	N	O	S	0	0	0
			2897	1852	475	553	17			

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			3	2	1		

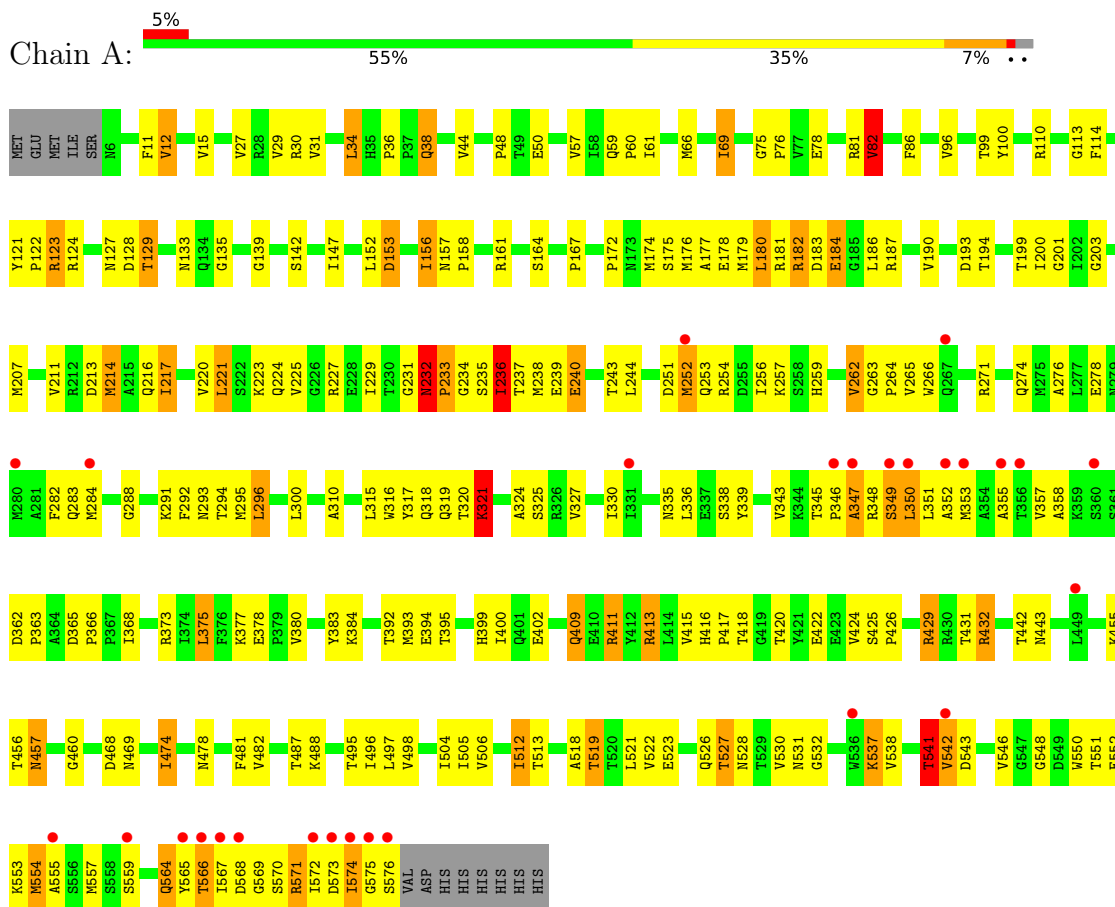
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total	O	0	0
			192	192		
5	D	86	Total	O	0	0
			86	86		

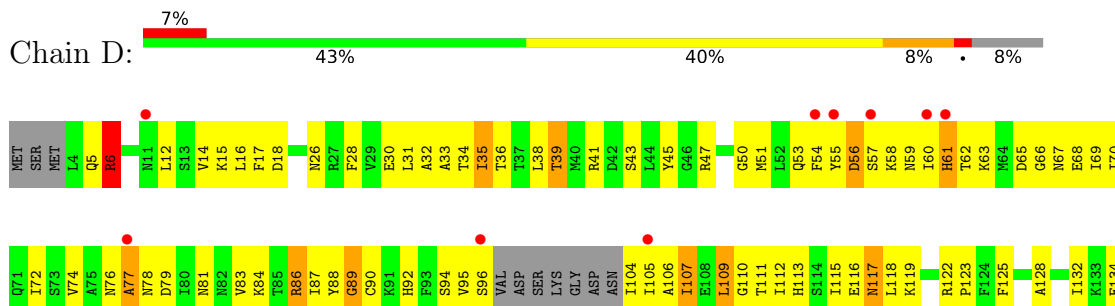
3 Residue-property plots

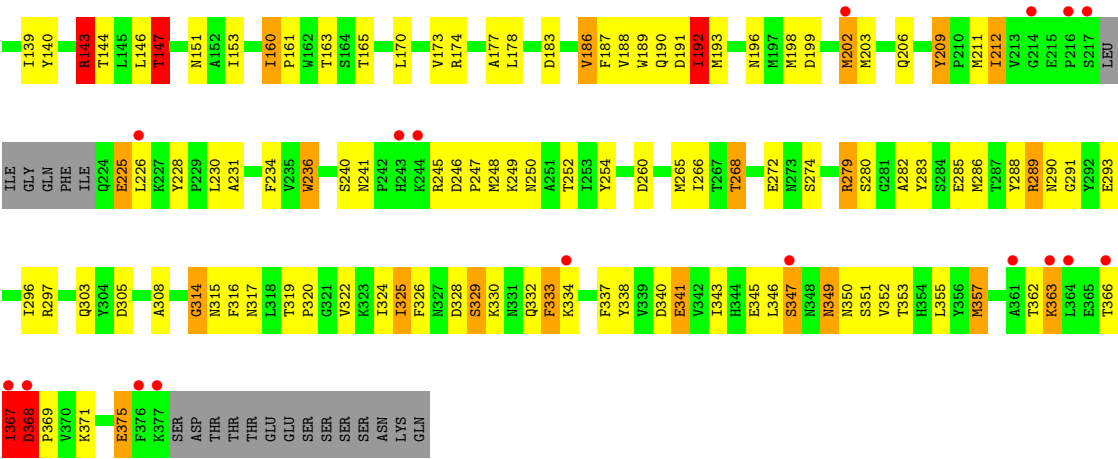
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Baseplate structural protein Gp27





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	137.13Å 137.13Å 396.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.55 – 2.80 47.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.55-2.80) 94.7 (47.55-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.86 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.281 0.229 , 0.285	Depositor DCC
R_{free} test set	3393 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, K

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	0.55	7/4479 (0.2%)	0.96	17/6074 (0.3%)
2	D	0.59	7/2964 (0.2%)	1.01	18/4018 (0.4%)
All	All	0.57	14/7443 (0.2%)	0.98	35/10092 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	192	ILE	C-O	-10.66	1.11	1.24
1	A	554	MET	C-N	-7.99	1.22	1.33
2	D	74	VAL	C-N	-7.23	1.24	1.33
1	A	12	VAL	C-N	-6.40	1.25	1.33
2	D	368	ASP	C-O	6.29	1.29	1.23
1	A	555	ALA	C-O	-6.16	1.16	1.24
1	A	235	SER	C-N	-5.94	1.25	1.33
2	D	192	ILE	C-N	5.92	1.42	1.33
2	D	347	SER	C-N	-5.84	1.25	1.33
2	D	367	ILE	C-O	5.72	1.30	1.24
1	A	236	ILE	C-N	-5.67	1.26	1.33
1	A	542	VAL	C-N	-5.32	1.26	1.33
2	D	89	GLY	C-N	-5.29	1.25	1.33
1	A	541	THR	C-N	-5.11	1.26	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ASN	CA-C-N	-9.49	107.97	119.84
1	A	232	ASN	C-N-CA	-9.49	107.97	119.84
2	D	192	ILE	CA-C-O	8.99	129.97	119.36
2	D	202	MET	CB-CA-C	-8.32	97.49	110.81
2	D	368	ASP	CB-CA-C	7.74	121.01	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	347	SER	CA-C-O	-7.63	112.73	121.58
2	D	147	THR	CA-C-N	7.21	127.66	120.52
2	D	147	THR	C-N-CA	7.21	127.66	120.52
1	A	236	ILE	CA-C-O	-6.87	113.20	120.76
1	A	262	VAL	N-CA-C	6.76	116.90	110.74
2	D	66	GLY	N-CA-C	-6.62	106.11	115.30
1	A	443	ASN	N-CA-C	6.41	118.35	111.36
1	A	432	ARG	CB-CA-C	6.27	121.01	110.79
1	A	12	VAL	CA-C-O	-6.25	113.07	121.32
2	D	363	LYS	N-CA-C	5.93	117.55	108.42
1	A	338	SER	N-CA-C	-5.92	104.90	111.71
1	A	542	VAL	CA-C-O	-5.90	113.41	120.78
1	A	82	VAL	N-CA-C	5.72	116.60	108.42
1	A	29	VAL	N-CA-C	5.69	116.31	108.12
2	D	151	ASN	CB-CA-C	5.62	121.07	111.68
1	A	69	ILE	CB-CA-C	-5.60	104.53	111.08
2	D	329	SER	N-CA-C	-5.57	106.49	113.28
1	A	236	ILE	CB-CA-C	5.30	119.88	110.71
2	D	143	ARG	CA-C-N	5.25	131.57	121.54
2	D	143	ARG	C-N-CA	5.25	131.57	121.54
2	D	165	THR	N-CA-C	5.12	117.46	110.55
2	D	209	TYR	CA-C-N	5.10	125.02	119.76
2	D	209	TYR	C-N-CA	5.10	125.02	119.76
1	A	541	THR	CA-C-N	5.08	131.12	121.97
1	A	541	THR	C-N-CA	5.08	131.12	121.97
2	D	367	ILE	O-C-N	-5.08	116.22	122.57
1	A	400	ILE	N-CA-C	5.06	115.40	108.12
2	D	279	ARG	N-CA-C	-5.02	104.46	110.88
1	A	86	PHE	CA-C-O	-5.02	114.99	120.36
2	D	186	VAL	N-CA-C	5.01	117.03	108.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4396	0	4310	281	0
2	D	2897	0	2828	180	0
3	A	1	0	0	0	0
4	A	3	0	0	0	1
5	A	192	0	0	11	0
5	D	86	0	0	5	0
All	All	7575	0	7138	459	1

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 32.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:ASN:ND2	2:D:350:ASN:H	1.60	0.99
1:A:552:GLU:HB2	1:A:554:MET:HE1	1.41	0.99
1:A:557:MET:HE2	1:A:559:SER:HB2	1.45	0.97
1:A:184:GLU:HG2	1:A:203:GLY:HA3	1.47	0.96
1:A:157:ASN:HD22	1:A:158:PRO:HD2	1.30	0.94
1:A:38:GLN:H	1:A:38:GLN:HE21	0.97	0.93
1:A:184:GLU:CG	1:A:203:GLY:HA3	1.98	0.93
1:A:384:LYS:HB2	1:A:409:GLN:HG2	1.52	0.91
1:A:133:ASN:HD21	1:A:392:THR:H	1.18	0.90
1:A:31:VAL:HB	1:A:34:LEU:HD11	1.52	0.90
1:A:541:THR:O	1:A:542:VAL:HG23	1.71	0.89
2:D:290:ASN:HD21	2:D:371:LYS:HA	1.34	0.88
2:D:153:ILE:HG21	2:D:202:MET:HE1	1.57	0.87
1:A:38:GLN:H	1:A:38:GLN:NE2	1.74	0.85
1:A:350:LEU:HD23	1:A:350:LEU:H	1.42	0.85
1:A:350:LEU:HD13	1:A:355:ALA:HB3	1.59	0.85
2:D:337:PHE:HB3	2:D:357:MET:HG3	1.60	0.84
2:D:41:ARG:HG3	2:D:343:ILE:HG13	1.60	0.84
1:A:38:GLN:HE21	1:A:38:GLN:N	1.76	0.83
1:A:237:THR:HG22	1:A:240:GLU:HB2	1.59	0.83
1:A:541:THR:HG22	1:A:542:VAL:H	1.43	0.82
1:A:237:THR:HG23	1:A:240:GLU:H	1.45	0.81
1:A:214:MET:HG3	1:A:232:ASN:O	1.81	0.80
1:A:31:VAL:HB	1:A:34:LEU:CD1	2.10	0.80
1:A:232:ASN:HB3	1:A:233:PRO:CD	2.12	0.80
1:A:251:ASP:HA	1:A:254:ARG:HH21	1.45	0.79
2:D:95:VAL:HA	2:D:105:ILE:HG22	1.64	0.78
1:A:288:GLY:O	1:A:291:LYS:HG2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:ASN:O	2:D:119:LYS:HD2	1.86	0.75
1:A:571:ARG:C	1:A:572:ILE:HD12	2.11	0.75
1:A:50:GLU:CD	1:A:50:GLU:H	1.94	0.74
1:A:214:MET:HE1	1:A:217:ILE:HG21	1.69	0.73
1:A:384:LYS:CB	1:A:409:GLN:HG2	2.18	0.73
2:D:153:ILE:CG2	2:D:202:MET:HE1	2.19	0.73
1:A:552:GLU:CB	1:A:554:MET:HE1	2.18	0.72
1:A:223:LYS:HE2	1:A:223:LYS:HA	1.69	0.72
1:A:350:LEU:HB3	1:A:355:ALA:HB2	1.72	0.72
1:A:552:GLU:HB2	1:A:554:MET:CE	2.20	0.71
1:A:237:THR:CG2	1:A:240:GLU:H	2.04	0.71
1:A:567:ILE:HG22	1:A:568:ASP:N	2.06	0.71
1:A:512:ILE:HD12	1:A:512:ILE:N	2.05	0.70
1:A:413:ARG:HD2	1:A:415:VAL:CG2	2.22	0.70
2:D:144:THR:O	2:D:147:THR:HG23	1.92	0.69
2:D:189:TRP:CH2	2:D:198:MET:HE3	2.28	0.69
2:D:59:ASN:O	2:D:62:THR:HG22	1.92	0.69
1:A:550:TRP:CD1	1:A:551:THR:N	2.60	0.69
2:D:86:ARG:NH1	2:D:192:ILE:HB	2.09	0.68
1:A:123:ARG:HD2	5:A:662:HOH:O	1.93	0.68
1:A:530:VAL:C	1:A:532:GLY:H	2.01	0.68
2:D:15:LYS:HE3	2:D:28:PHE:CE2	2.28	0.68
1:A:184:GLU:HG3	1:A:203:GLY:HA3	1.76	0.67
2:D:90:CYS:HA	2:D:107:ILE:HD11	1.75	0.67
2:D:110:GLY:HA3	2:D:115:ILE:HD11	1.76	0.67
2:D:31:LEU:C	2:D:33:ALA:H	2.03	0.67
2:D:366:THR:O	2:D:368:ASP:N	2.28	0.67
2:D:193:MET:HE2	2:D:193:MET:HA	1.74	0.67
1:A:573:ASP:C	1:A:574:ILE:HD12	2.20	0.66
2:D:349:ASN:ND2	2:D:350:ASN:N	2.38	0.66
1:A:190:VAL:HG21	1:A:214:MET:HE1	1.78	0.65
2:D:189:TRP:HH2	2:D:198:MET:HE3	1.62	0.65
1:A:232:ASN:O	1:A:234:GLY:N	2.29	0.65
2:D:240:SER:HB3	2:D:245:ARG:HH12	1.61	0.65
1:A:495:THR:C	1:A:496:ILE:HD12	2.22	0.65
1:A:567:ILE:HG22	1:A:568:ASP:H	1.61	0.65
2:D:5:GLN:HB3	2:D:6:ARG:HH11	1.61	0.65
2:D:34:THR:HB	2:D:55:TYR:O	1.97	0.65
2:D:140:TYR:CB	2:D:147:THR:HG22	2.26	0.64
1:A:232:ASN:HB3	1:A:233:PRO:HD3	1.77	0.64
2:D:347:SER:HB3	2:D:349:ASN:ND2	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:O	1:A:474:ILE:HG13	1.95	0.64
2:D:53:GLN:HB3	2:D:106:ALA:HB2	1.79	0.64
1:A:550:TRP:CD1	1:A:551:THR:H	2.16	0.64
2:D:366:THR:O	2:D:369:PRO:HD3	1.98	0.63
1:A:221:LEU:HB3	1:A:229:ILE:HD12	1.80	0.63
1:A:569:GLY:C	1:A:571:ARG:H	2.06	0.62
1:A:176:MET:HG3	1:A:278:GLU:OE2	1.99	0.62
1:A:190:VAL:HG21	1:A:214:MET:CE	2.28	0.62
1:A:251:ASP:HA	1:A:254:ARG:NH2	2.12	0.62
1:A:522:VAL:O	1:A:522:VAL:HG23	1.99	0.62
1:A:61:ILE:C	1:A:61:ILE:HD12	2.25	0.62
1:A:177:ALA:O	1:A:181:ARG:HB2	2.00	0.62
1:A:574:ILE:HD12	1:A:574:ILE:N	2.14	0.61
1:A:152:LEU:HD22	1:A:378:GLU:HG2	1.81	0.61
2:D:86:ARG:HH11	2:D:192:ILE:HB	1.66	0.61
1:A:44:VAL:O	2:D:122:ARG:HG2	2.01	0.61
2:D:86:ARG:HG3	2:D:87:ILE:N	2.13	0.61
1:A:564:GLN:HA	1:A:564:GLN:HE21	1.65	0.61
2:D:123:PRO:HA	2:D:161:PRO:HA	1.83	0.61
1:A:375:LEU:CD2	1:A:455:LYS:HD3	2.31	0.60
1:A:350:LEU:HB2	1:A:355:ALA:H	1.65	0.60
2:D:16:LEU:HD12	2:D:16:LEU:O	2.01	0.60
1:A:541:THR:O	1:A:542:VAL:CG2	2.47	0.60
1:A:237:THR:HG22	1:A:240:GLU:CD	2.26	0.60
1:A:292:PHE:O	1:A:296:LEU:HB2	2.01	0.60
1:A:330:ILE:HD12	1:A:336:LEU:HD12	1.84	0.60
1:A:213:ASP:O	1:A:217:ILE:HG12	2.02	0.60
1:A:350:LEU:HB3	1:A:355:ALA:CB	2.31	0.60
1:A:542:VAL:HG12	1:A:543:ASP:N	2.17	0.60
2:D:6:ARG:CD	2:D:6:ARG:N	2.65	0.60
2:D:35:ILE:HD13	2:D:35:ILE:O	2.02	0.60
2:D:250:ASN:HD21	2:D:272:GLU:HB2	1.67	0.60
2:D:314:GLY:HA3	2:D:351:SER:OG	2.01	0.60
2:D:367:ILE:HG22	2:D:367:ILE:O	2.02	0.60
1:A:416:HIS:CE1	1:A:418:THR:HG23	2.37	0.59
2:D:349:ASN:H	2:D:349:ASN:HD22	1.50	0.59
1:A:350:LEU:CB	1:A:355:ALA:H	2.14	0.59
1:A:395:THR:OG1	1:A:399:HIS:HB2	2.03	0.59
1:A:36:PRO:HB2	1:A:38:GLN:NE2	2.17	0.59
1:A:200:ILE:HG12	1:A:201:GLY:H	1.67	0.59
1:A:330:ILE:HD13	1:A:335:ASN:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ARG:HB3	2:D:146:LEU:HD12	1.85	0.59
2:D:170:LEU:HD22	2:D:188:VAL:HG11	1.84	0.59
2:D:95:VAL:HA	2:D:105:ILE:CG2	2.33	0.58
2:D:153:ILE:HG21	2:D:202:MET:CE	2.32	0.58
1:A:375:LEU:HD22	1:A:455:LYS:HD3	1.85	0.58
2:D:252:THR:HG21	2:D:265:MET:HE3	1.84	0.58
1:A:237:THR:HG22	1:A:240:GLU:CB	2.30	0.58
1:A:526:GLN:C	1:A:527:THR:HG22	2.27	0.58
1:A:152:LEU:HD11	1:A:380:VAL:HG12	1.84	0.58
1:A:176:MET:O	1:A:180:LEU:HB2	2.04	0.58
2:D:104:ILE:HG23	2:D:104:ILE:O	2.04	0.58
2:D:160:ILE:HD13	2:D:160:ILE:H	1.68	0.58
1:A:186:LEU:C	1:A:187:ARG:HD2	2.29	0.58
1:A:213:ASP:OD2	1:A:216:GLN:HG3	2.04	0.58
1:A:424:VAL:HA	1:A:429:ARG:O	2.04	0.57
2:D:119:LYS:HG3	5:D:530:HOH:O	2.04	0.57
2:D:290:ASN:ND2	2:D:371:LYS:HA	2.14	0.57
1:A:48:PRO:HB2	1:A:50:GLU:OE2	2.04	0.57
2:D:35:ILE:HD13	2:D:35:ILE:C	2.29	0.57
2:D:211:MET:HE2	2:D:231:ALA:HB2	1.87	0.57
2:D:38:LEU:HD23	2:D:346:LEU:HD11	1.86	0.57
2:D:128:ALA:O	2:D:132:ILE:HG13	2.04	0.57
1:A:564:GLN:HA	1:A:564:GLN:NE2	2.20	0.57
1:A:12:VAL:CG1	1:A:100:TYR:OH	2.53	0.57
2:D:56:ASP:OD1	2:D:57:SER:N	2.37	0.57
1:A:257:LYS:HE3	1:A:266:TRP:CH2	2.40	0.57
1:A:231:GLY:HA2	5:A:692:HOH:O	2.04	0.56
1:A:537:LYS:HE3	1:A:537:LYS:O	2.05	0.56
2:D:5:GLN:HG3	5:D:499:HOH:O	2.06	0.56
1:A:157:ASN:HD22	1:A:158:PRO:CD	2.14	0.56
1:A:12:VAL:HG11	1:A:100:TYR:OH	2.05	0.56
1:A:174:MET:HE3	1:A:179:MET:HB2	1.88	0.56
1:A:237:THR:HG21	5:A:640:HOH:O	2.04	0.56
1:A:522:VAL:HG21	1:A:526:GLN:HB2	1.88	0.56
2:D:60:ILE:HD12	2:D:63:LYS:HD3	1.88	0.56
2:D:31:LEU:O	2:D:33:ALA:N	2.39	0.56
2:D:174:ARG:NH1	2:D:188:VAL:O	2.39	0.56
2:D:51:MET:HE1	2:D:106:ALA:HB1	1.87	0.55
1:A:167:PRO:HG3	1:A:343:VAL:HG11	1.87	0.55
1:A:564:GLN:HG3	1:A:565:TYR:N	2.20	0.55
1:A:186:LEU:O	1:A:187:ARG:HD2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ALA:HB2	1:A:330:ILE:HG21	1.88	0.55
1:A:526:GLN:HG2	1:A:527:THR:N	2.22	0.55
1:A:12:VAL:HG12	5:A:621:HOH:O	2.06	0.55
2:D:17:PHE:CE2	2:D:28:PHE:HB3	2.42	0.55
1:A:174:MET:HE2	1:A:336:LEU:HD23	1.88	0.55
2:D:241:ASN:C	2:D:241:ASN:HD22	2.15	0.55
2:D:58:LYS:NZ	2:D:58:LYS:HB3	2.22	0.54
2:D:212:ILE:HD13	2:D:230:LEU:HA	1.89	0.54
2:D:283:TYR:O	2:D:286:MET:HG2	2.07	0.54
1:A:253:GLN:O	1:A:256:ILE:HG22	2.07	0.54
1:A:413:ARG:HD2	1:A:415:VAL:HG23	1.88	0.54
2:D:173:VAL:HG13	2:D:177:ALA:CB	2.37	0.54
2:D:5:GLN:HB3	2:D:6:ARG:NH1	2.23	0.54
2:D:248:MET:O	2:D:268:THR:HG21	2.07	0.54
1:A:214:MET:HG2	1:A:232:ASN:OD1	2.08	0.54
2:D:283:TYR:C	2:D:285:GLU:H	2.15	0.54
1:A:456:THR:HG22	1:A:457:ASN:N	2.23	0.54
1:A:139:GLY:O	1:A:142:SER:HB3	2.08	0.54
1:A:321:LYS:HB2	1:A:460:GLY:CA	2.38	0.54
2:D:212:ILE:HG13	2:D:226:LEU:HD22	1.90	0.54
2:D:349:ASN:CG	2:D:350:ASN:H	2.14	0.54
1:A:11:PHE:CD1	1:A:11:PHE:C	2.86	0.54
2:D:95:VAL:HG13	2:D:105:ILE:CG2	2.39	0.53
1:A:221:LEU:HD13	1:A:229:ILE:HD13	1.89	0.53
1:A:564:GLN:HG3	1:A:565:TYR:H	1.73	0.53
2:D:45:TYR:HE2	2:D:340:ASP:OD2	1.91	0.53
1:A:180:LEU:HD21	1:A:282:PHE:CG	2.44	0.53
1:A:164:SER:HB3	5:A:636:HOH:O	2.08	0.53
1:A:368:ILE:HD12	1:A:368:ILE:N	2.22	0.53
1:A:496:ILE:HG22	1:A:497:LEU:N	2.23	0.53
1:A:236:ILE:HG13	1:A:240:GLU:HB3	1.91	0.53
1:A:357:VAL:HG12	1:A:357:VAL:O	2.08	0.53
2:D:349:ASN:HD22	2:D:349:ASN:N	2.04	0.53
1:A:474:ILE:HD11	1:A:478:ASN:HB2	1.91	0.53
2:D:77:ALA:O	2:D:78:ASN:C	2.52	0.53
1:A:365:ASP:HB3	1:A:366:PRO:HD2	1.90	0.53
1:A:384:LYS:HB2	1:A:409:GLN:CG	2.33	0.53
1:A:425:SER:HB2	1:A:426:PRO:HD2	1.91	0.53
1:A:318:GLN:O	1:A:321:LYS:HD2	2.09	0.52
1:A:127:ASN:ND2	1:A:129:THR:HG23	2.23	0.52
1:A:38:GLN:NE2	1:A:38:GLN:N	2.47	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLN:HG3	5:A:651:HOH:O	2.07	0.52
1:A:174:MET:HE1	1:A:339:TYR:CD1	2.44	0.52
2:D:18:ASP:HA	2:D:68:GLU:HG3	1.90	0.52
2:D:95:VAL:HG13	2:D:105:ILE:HG22	1.91	0.52
2:D:189:TRP:CD1	2:D:320:PRO:HG2	2.45	0.52
1:A:127:ASN:CG	1:A:129:THR:HG23	2.35	0.52
1:A:350:LEU:HD12	1:A:353:MET:HA	1.92	0.52
2:D:349:ASN:HD22	2:D:350:ASN:H	1.54	0.52
1:A:265:VAL:HG21	1:A:296:LEU:HG	1.92	0.52
1:A:321:LYS:HB2	1:A:460:GLY:HA2	1.91	0.52
1:A:353:MET:O	1:A:357:VAL:HG23	2.09	0.52
1:A:266:TRP:CD1	1:A:274:GLN:HG2	2.44	0.51
2:D:203:MET:O	2:D:206:GLN:HB2	2.10	0.51
1:A:541:THR:C	1:A:542:VAL:HG23	2.35	0.51
2:D:325:ILE:HD13	2:D:325:ILE:C	2.35	0.51
1:A:15:VAL:HG13	1:A:27:VAL:HB	1.92	0.51
1:A:383:TYR:O	1:A:384:LYS:HG3	2.08	0.51
2:D:345:GLU:HB3	2:D:352:VAL:HG23	1.92	0.51
1:A:239:GLU:CD	1:A:239:GLU:H	2.19	0.51
1:A:133:ASN:HD21	1:A:392:THR:N	1.97	0.51
1:A:113:GLY:O	1:A:114:PHE:HB2	2.10	0.51
1:A:295:MET:HB2	1:A:310:ALA:CB	2.40	0.51
1:A:512:ILE:N	1:A:512:ILE:CD1	2.71	0.51
2:D:113:HIS:HB3	2:D:139:ILE:HG21	1.93	0.51
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.75	0.51
1:A:568:ASP:CG	1:A:569:GLY:H	2.18	0.51
1:A:34:LEU:HD22	2:D:163:THR:HG21	1.92	0.51
1:A:567:ILE:CG2	1:A:568:ASP:H	2.24	0.51
2:D:209:TYR:HB3	2:D:324:ILE:HD13	1.93	0.51
1:A:259:HIS:HB3	1:A:262:VAL:HB	1.92	0.51
1:A:156:ILE:C	1:A:156:ILE:HD12	2.36	0.50
2:D:36:THR:OG1	2:D:104:ILE:HD11	2.11	0.50
2:D:189:TRP:CZ3	2:D:198:MET:HG2	2.46	0.50
1:A:295:MET:HB2	1:A:310:ALA:HB3	1.93	0.50
1:A:276:ALA:HB2	1:A:330:ILE:CG2	2.42	0.50
1:A:346:PRO:C	1:A:348:ARG:H	2.20	0.50
1:A:157:ASN:ND2	1:A:158:PRO:HD2	2.12	0.50
2:D:178:LEU:HD13	2:D:178:LEU:C	2.37	0.50
2:D:225:GLU:O	2:D:225:GLU:HG3	2.11	0.50
1:A:207:MET:SD	1:A:211:VAL:HG21	2.52	0.50
1:A:392:THR:HG23	1:A:402:GLU:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:TRP:HD1	1:A:551:THR:N	2.08	0.50
1:A:574:ILE:HG22	1:A:574:ILE:O	2.11	0.50
1:A:200:ILE:HG12	1:A:201:GLY:N	2.26	0.50
1:A:350:LEU:HD23	1:A:350:LEU:N	2.21	0.50
1:A:504:ILE:O	1:A:505:ILE:HD13	2.12	0.50
2:D:107:ILE:HD13	2:D:107:ILE:C	2.37	0.50
1:A:57:VAL:HG12	1:A:96:VAL:HB	1.93	0.50
2:D:375:GLU:H	2:D:375:GLU:CD	2.20	0.49
1:A:243:THR:O	1:A:244:LEU:C	2.55	0.49
1:A:350:LEU:HG	1:A:353:MET:HE3	1.94	0.49
2:D:140:TYR:CD1	2:D:143:ARG:NH2	2.79	0.49
2:D:43:SER:HA	2:D:341:GLU:HB2	1.94	0.49
2:D:16:LEU:HD12	2:D:16:LEU:C	2.37	0.49
2:D:53:GLN:HB3	2:D:106:ALA:CB	2.40	0.49
2:D:107:ILE:CD1	2:D:109:LEU:HD12	2.42	0.49
1:A:512:ILE:HD12	1:A:512:ILE:H	1.74	0.49
1:A:530:VAL:C	1:A:532:GLY:N	2.66	0.49
2:D:53:GLN:HA	2:D:106:ALA:HA	1.93	0.49
2:D:56:ASP:OD2	2:D:60:ILE:HG22	2.12	0.49
1:A:135:GLY:HA2	1:A:383:TYR:OH	2.13	0.49
1:A:214:MET:HE1	1:A:217:ILE:CG2	2.39	0.49
1:A:530:VAL:O	1:A:532:GLY:N	2.46	0.49
1:A:574:ILE:O	1:A:576:SER:N	2.46	0.49
2:D:6:ARG:N	2:D:6:ARG:HD2	2.26	0.49
2:D:186:VAL:HG12	2:D:187:PHE:N	2.26	0.49
1:A:34:LEU:HD12	1:A:34:LEU:H	1.77	0.49
1:A:542:VAL:O	1:A:543:ASP:HB2	2.11	0.49
2:D:54:PHE:N	2:D:54:PHE:CD1	2.80	0.49
1:A:542:VAL:CG1	1:A:543:ASP:N	2.76	0.48
2:D:349:ASN:ND2	2:D:349:ASN:H	2.11	0.48
1:A:256:ILE:HG23	1:A:257:LYS:N	2.28	0.48
1:A:496:ILE:CG2	1:A:497:LEU:N	2.76	0.48
2:D:325:ILE:HD13	2:D:326:PHE:N	2.28	0.48
2:D:375:GLU:CD	2:D:375:GLU:N	2.71	0.48
1:A:324:ALA:HA	1:A:327:VAL:HG22	1.94	0.48
2:D:41:ARG:HG3	2:D:343:ILE:CG1	2.38	0.48
2:D:315:ASN:ND2	2:D:317:ASN:H	2.11	0.48
1:A:82:VAL:HG22	1:A:96:VAL:HG13	1.95	0.48
1:A:121:TYR:HA	1:A:122:PRO:C	2.39	0.48
1:A:474:ILE:CD1	1:A:478:ASN:HB2	2.44	0.48
1:A:546:VAL:HG22	1:A:548:GLY:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:HH11	1:A:431:THR:CB	2.26	0.48
2:D:79:ASP:C	2:D:81:ASN:N	2.71	0.48
1:A:257:LYS:HG2	1:A:266:TRP:CZ3	2.49	0.48
1:A:351:LEU:O	1:A:352:ALA:HB3	2.13	0.47
2:D:303:GLN:OE1	2:D:363:LYS:HD2	2.14	0.47
1:A:81:ARG:NH2	1:A:128:ASP:OD1	2.45	0.47
1:A:179:MET:HE2	1:A:339:TYR:CZ	2.49	0.47
1:A:199:THR:HG22	1:A:200:ILE:N	2.29	0.47
1:A:175:SER:HB3	1:A:178:GLU:HG3	1.96	0.47
1:A:252:MET:HE2	1:A:253:GLN:HA	1.97	0.47
1:A:345:THR:C	1:A:347:ALA:H	2.22	0.47
1:A:362:ASP:OD1	1:A:363:PRO:HD2	2.14	0.47
2:D:190:GLN:HG3	5:D:536:HOH:O	2.15	0.47
2:D:349:ASN:CG	2:D:350:ASN:N	2.72	0.47
1:A:512:ILE:CD1	1:A:512:ILE:H	2.27	0.47
1:A:176:MET:HE2	1:A:278:GLU:CB	2.45	0.47
1:A:225:VAL:HG11	1:A:236:ILE:HD11	1.96	0.47
2:D:140:TYR:HB3	2:D:147:THR:HG22	1.95	0.47
2:D:279:ARG:HG3	2:D:289:ARG:O	2.14	0.47
2:D:338:TYR:O	2:D:357:MET:HB2	2.14	0.47
1:A:383:TYR:CD2	1:A:411:ARG:NH1	2.83	0.47
1:A:538:VAL:HG11	1:A:541:THR:O	2.15	0.47
2:D:345:GLU:HB3	2:D:352:VAL:CG2	2.45	0.47
1:A:66:MET:O	1:A:69:ILE:HG12	2.15	0.47
1:A:167:PRO:CG	1:A:343:VAL:HG11	2.44	0.47
1:A:373:ARG:HA	1:A:373:ARG:HE	1.80	0.46
2:D:315:ASN:ND2	2:D:315:ASN:C	2.72	0.46
1:A:481:PHE:CD1	1:A:481:PHE:C	2.93	0.46
1:A:512:ILE:HG22	1:A:513:THR:N	2.29	0.46
1:A:214:MET:HE2	1:A:234:GLY:H	1.81	0.46
2:D:95:VAL:CA	2:D:105:ILE:HG22	2.39	0.46
2:D:246:ASP:N	2:D:247:PRO:CD	2.78	0.46
1:A:330:ILE:CD1	1:A:336:LEU:HA	2.45	0.46
1:A:317:TYR:HE2	1:A:325:SER:HA	1.81	0.46
1:A:429:ARG:HH11	1:A:431:THR:HB	1.79	0.46
1:A:569:GLY:C	1:A:571:ARG:N	2.73	0.46
2:D:199:ASP:OD2	2:D:202:MET:HG3	2.15	0.46
2:D:268:THR:HG22	2:D:268:THR:O	2.14	0.46
1:A:526:GLN:NE2	1:A:528:ASN:HD21	2.14	0.46
1:A:237:THR:CG2	1:A:240:GLU:HB2	2.39	0.46
1:A:349:SER:HB2	1:A:350:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:GLU:C	1:A:553:LYS:HD2	2.40	0.46
1:A:564:GLN:HE21	1:A:564:GLN:CA	2.26	0.46
1:A:184:GLU:CG	1:A:203:GLY:CA	2.85	0.46
2:D:112:ILE:HG22	2:D:113:HIS:N	2.31	0.46
2:D:212:ILE:HD12	2:D:228:TYR:O	2.16	0.46
1:A:176:MET:HE2	1:A:278:GLU:HB2	1.98	0.45
1:A:227:ARG:HG2	5:A:770:HOH:O	2.14	0.45
1:A:220:VAL:O	1:A:224:GLN:HG3	2.16	0.45
1:A:223:LYS:HE3	5:A:661:HOH:O	2.16	0.45
2:D:76:ASN:HB3	2:D:316:PHE:CD1	2.51	0.45
1:A:567:ILE:CG2	1:A:568:ASP:N	2.74	0.45
2:D:212:ILE:CD1	2:D:230:LEU:HA	2.45	0.45
2:D:283:TYR:C	2:D:285:GLU:N	2.71	0.45
1:A:59:GLN:HB3	1:A:60:PRO:HD2	1.97	0.45
2:D:160:ILE:HG21	2:D:282:ALA:HB1	1.98	0.45
2:D:206:GLN:OE1	2:D:322:VAL:HA	2.16	0.45
2:D:212:ILE:HD11	2:D:226:LEU:HD13	1.98	0.45
2:D:325:ILE:O	2:D:325:ILE:HG23	2.16	0.45
1:A:239:GLU:O	1:A:240:GLU:C	2.60	0.45
1:A:265:VAL:HA	1:A:300:LEU:HD21	1.98	0.45
2:D:328:ASP:CG	2:D:329:SER:H	2.25	0.45
2:D:43:SER:HB3	2:D:47:ARG:HB3	1.99	0.45
2:D:51:MET:HE1	2:D:53:GLN:HB3	1.98	0.45
2:D:346:LEU:C	2:D:346:LEU:HD12	2.41	0.45
1:A:182:ARG:HG3	1:A:183:ASP:N	2.32	0.45
2:D:72:ILE:HD12	2:D:88:TYR:CE1	2.52	0.45
1:A:572:ILE:HD12	1:A:572:ILE:N	2.31	0.45
2:D:95:VAL:HG22	2:D:105:ILE:HG21	1.99	0.44
2:D:245:ARG:HD2	5:D:478:HOH:O	2.17	0.44
1:A:34:LEU:HD13	1:A:34:LEU:C	2.43	0.44
2:D:330:LYS:O	2:D:330:LYS:HG3	2.17	0.44
1:A:123:ARG:NH2	5:A:596:HOH:O	2.50	0.44
1:A:172:PRO:HB2	1:A:336:LEU:HD22	1.98	0.44
1:A:251:ASP:O	1:A:254:ARG:HG2	2.16	0.44
2:D:319:THR:O	2:D:322:VAL:HG13	2.18	0.44
1:A:30:ARG:HG3	1:A:30:ARG:NH2	2.33	0.44
1:A:253:GLN:C	1:A:256:ILE:HG22	2.43	0.44
2:D:315:ASN:C	2:D:315:ASN:HD22	2.24	0.44
2:D:367:ILE:O	2:D:367:ILE:CG2	2.65	0.44
1:A:161:ARG:NH1	1:A:167:PRO:HD2	2.32	0.44
1:A:557:MET:HE2	1:A:559:SER:CB	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ASN:ND2	2:D:272:GLU:HB2	2.33	0.44
1:A:81:ARG:HG2	5:A:609:HOH:O	2.17	0.44
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.81	0.44
1:A:283:GLN:NE2	1:A:316:TRP:HE1	2.15	0.44
1:A:123:ARG:O	1:A:124:ARG:HB3	2.18	0.44
1:A:216:GLN:O	1:A:217:ILE:C	2.61	0.44
1:A:541:THR:CG2	1:A:542:VAL:H	2.14	0.44
1:A:554:MET:N	1:A:554:MET:HE3	2.33	0.44
1:A:82:VAL:HG23	1:A:99:THR:HG22	2.00	0.43
1:A:252:MET:HE1	1:A:278:GLU:HG2	2.00	0.43
1:A:348:ARG:HD3	1:A:349:SER:H	1.82	0.43
1:A:352:ALA:O	1:A:353:MET:HB2	2.18	0.43
1:A:518:ALA:C	1:A:519:THR:HG22	2.43	0.43
2:D:12:LEU:HD11	2:D:14:VAL:CG2	2.48	0.43
2:D:245:ARG:HD3	2:D:305:ASP:CG	2.43	0.43
1:A:251:ASP:CA	1:A:254:ARG:NH2	2.81	0.43
2:D:191:ASP:CB	2:D:193:MET:H	2.31	0.43
2:D:236:TRP:CD1	2:D:308:ALA:HB2	2.53	0.43
1:A:262:VAL:O	1:A:263:GLY:C	2.61	0.43
1:A:550:TRP:NE1	1:A:552:GLU:OE2	2.52	0.43
2:D:260:ASP:OD1	2:D:289:ARG:NH2	2.51	0.43
1:A:184:GLU:HG3	1:A:203:GLY:CA	2.47	0.43
1:A:252:MET:HE1	1:A:278:GLU:CG	2.49	0.43
1:A:393:MET:HG2	1:A:394:GLU:N	2.32	0.43
2:D:31:LEU:C	2:D:33:ALA:N	2.69	0.43
2:D:332:GLN:O	2:D:332:GLN:HG2	2.19	0.43
1:A:263:GLY:N	1:A:264:PRO:HD2	2.34	0.43
1:A:284:MET:HE1	1:A:316:TRP:CD1	2.54	0.43
2:D:111:THR:O	2:D:115:ILE:HG12	2.18	0.43
1:A:425:SER:OG	1:A:429:ARG:HB3	2.18	0.43
1:A:416:HIS:CG	1:A:417:PRO:HD2	2.53	0.43
1:A:232:ASN:O	1:A:233:PRO:C	2.56	0.42
1:A:315:LEU:O	1:A:319:GLN:HG2	2.19	0.42
2:D:240:SER:CB	2:D:245:ARG:HH12	2.29	0.42
1:A:236:ILE:HD12	1:A:236:ILE:HA	1.92	0.42
1:A:553:LYS:C	1:A:554:MET:HE3	2.44	0.42
2:D:107:ILE:HD12	2:D:109:LEU:HD12	2.01	0.42
1:A:81:ARG:HB3	1:A:100:TYR:CZ	2.55	0.42
1:A:350:LEU:H	1:A:350:LEU:CD2	2.23	0.42
1:A:383:TYR:CD1	1:A:383:TYR:C	2.96	0.42
2:D:349:ASN:HD22	2:D:350:ASN:N	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HG2	1:A:349:SER:N	2.35	0.42
1:A:526:GLN:HE21	1:A:528:ASN:HD21	1.67	0.42
2:D:6:ARG:HD2	2:D:6:ARG:H	1.84	0.42
1:A:574:ILE:N	1:A:574:ILE:CD1	2.82	0.42
2:D:89:GLY:N	2:D:112:ILE:HD12	2.34	0.42
1:A:221:LEU:O	1:A:225:VAL:HG22	2.19	0.42
2:D:34:THR:CB	2:D:55:TYR:O	2.67	0.42
1:A:346:PRO:C	1:A:348:ARG:N	2.77	0.42
2:D:186:VAL:CG1	2:D:187:PHE:N	2.83	0.42
2:D:189:TRP:CE2	2:D:196:ASN:HB2	2.55	0.42
1:A:225:VAL:HG12	1:A:244:LEU:HD11	2.02	0.42
2:D:334:LYS:HD2	2:D:334:LYS:HA	1.87	0.42
2:D:254:TYR:CE2	2:D:274:SER:HB2	2.54	0.42
1:A:293:ASN:O	1:A:294:THR:C	2.63	0.41
1:A:422:GLU:HA	1:A:431:THR:O	2.20	0.41
1:A:566:THR:OG1	1:A:567:ILE:N	2.53	0.41
2:D:125:PHE:CE1	2:D:134:GLU:HG3	2.54	0.41
2:D:94:SER:O	2:D:105:ILE:HB	2.20	0.41
1:A:75:GLY:N	1:A:76:PRO:HD2	2.35	0.41
1:A:256:ILE:CG2	1:A:257:LYS:N	2.82	0.41
1:A:324:ALA:O	1:A:327:VAL:HG22	2.20	0.41
1:A:474:ILE:HD11	1:A:478:ASN:N	2.36	0.41
1:A:568:ASP:CG	1:A:569:GLY:N	2.77	0.41
2:D:234:PHE:HE1	2:D:326:PHE:CE1	2.38	0.41
2:D:5:GLN:HB3	2:D:6:ARG:HD2	2.02	0.41
2:D:45:TYR:CE2	2:D:340:ASP:OD2	2.71	0.41
1:A:225:VAL:HG21	1:A:236:ILE:HD11	2.01	0.41
2:D:39:THR:O	2:D:50:GLY:CA	2.68	0.41
2:D:353:THR:HG22	2:D:355:LEU:CD1	2.50	0.41
1:A:110:ARG:NH2	5:A:766:HOH:O	2.53	0.41
1:A:266:TRP:CE2	1:A:274:GLN:CD	2.99	0.41
1:A:320:THR:O	1:A:320:THR:HG22	2.21	0.41
1:A:565:TYR:C	1:A:566:THR:HG22	2.46	0.41
1:A:186:LEU:HD21	1:A:238:MET:SD	2.61	0.41
1:A:207:MET:CE	1:A:220:VAL:HG21	2.51	0.41
1:A:468:ASP:CG	1:A:469:ASN:H	2.27	0.41
2:D:84:LYS:HE3	2:D:193:MET:SD	2.61	0.41
2:D:92:HIS:ND1	2:D:92:HIS:C	2.79	0.41
2:D:266:ILE:HD12	2:D:291:GLY:C	2.46	0.41
2:D:297:ARG:HD3	5:D:419:HOH:O	2.20	0.41
2:D:346:LEU:HD12	2:D:346:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:SER:C	2:D:349:ASN:H	2.28	0.41
1:A:153:ASP:O	1:A:377:LYS:HG3	2.21	0.41
1:A:227:ARG:HH21	1:A:229:ILE:HG12	1.86	0.41
2:D:96:SER:OG	2:D:104:ILE:N	2.54	0.41
2:D:288:TYR:CE2	2:D:371:LYS:HD2	2.56	0.41
2:D:347:SER:C	2:D:349:ASN:N	2.79	0.41
1:A:474:ILE:O	1:A:474:ILE:CG1	2.65	0.40
2:D:16:LEU:HA	2:D:69:ILE:O	2.21	0.40
2:D:70:ILE:N	2:D:70:ILE:HD12	2.37	0.40
2:D:241:ASN:C	2:D:241:ASN:ND2	2.79	0.40
2:D:293:GLU:HA	2:D:296:ILE:HG22	2.02	0.40
2:D:333:PHE:CD1	2:D:333:PHE:N	2.89	0.40
1:A:30:ARG:HG3	1:A:30:ARG:HH21	1.85	0.40
1:A:30:ARG:NE	1:A:113:GLY:HA3	2.35	0.40
2:D:160:ILE:HG21	2:D:282:ALA:CB	2.52	0.40
1:A:193:ASP:OD2	1:A:193:ASP:C	2.64	0.40
1:A:232:ASN:CB	1:A:233:PRO:CD	2.91	0.40
1:A:564:GLN:CG	1:A:565:TYR:H	2.34	0.40
2:D:61:HIS:ND1	2:D:61:HIS:C	2.80	0.40
2:D:249:LYS:O	2:D:268:THR:HG23	2.21	0.40
2:D:366:THR:C	2:D:368:ASP:H	2.28	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:586:PO4:P	4:A:586:PO4:O2[2_555]	1.50	0.70

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/584 (97%)	483 (85%)	72 (13%)	14 (2%)	4	16
2	D	355/391 (91%)	300 (84%)	46 (13%)	9 (2%)	4	16
All	All	924/975 (95%)	783 (85%)	118 (13%)	23 (2%)	4	16

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
2	D	117	ASN
2	D	367	ILE
1	A	321	LYS
1	A	349	SER
1	A	519	THR
1	A	531	ASN
1	A	571	ARG
1	A	575	GLY
2	D	6	ARG
2	D	32	ALA
2	D	225	GLU
2	D	314	GLY
2	D	26	ASN
2	D	77	ALA
1	A	347	ALA
1	A	358	ALA
1	A	521	LEU
2	D	56	ASP
1	A	564	GLN
1	A	570	SER
1	A	233	PRO
1	A	217	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	481/494 (97%)	437 (91%)	44 (9%)	9	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	322/350 (92%)	291 (90%)	31 (10%)	8	26
All	All	803/844 (95%)	728 (91%)	75 (9%)	8	27

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	38	GLN
1	A	78	GLU
1	A	82	VAL
1	A	123	ARG
1	A	129	THR
1	A	147	ILE
1	A	153	ASP
1	A	156	ILE
1	A	180	LEU
1	A	182	ARG
1	A	184	GLU
1	A	194	THR
1	A	214	MET
1	A	221	LEU
1	A	236	ILE
1	A	240	GLU
1	A	252	MET
1	A	271	ARG
1	A	296	LEU
1	A	321	LYS
1	A	350	LEU
1	A	375	LEU
1	A	409	GLN
1	A	411	ARG
1	A	413	ARG
1	A	420	THR
1	A	429	ARG
1	A	432	ARG
1	A	442	THR
1	A	457	ASN
1	A	474	ILE
1	A	482	VAL
1	A	487	THR
1	A	488	LYS
1	A	498	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	506	VAL
1	A	512	ILE
1	A	523	GLU
1	A	527	THR
1	A	537	LYS
1	A	541	THR
1	A	566	THR
1	A	574	ILE
2	D	6	ARG
2	D	30	GLU
2	D	35	ILE
2	D	39	THR
2	D	61	HIS
2	D	65	ASP
2	D	67	ASN
2	D	83	VAL
2	D	86	ARG
2	D	107	ILE
2	D	109	LEU
2	D	116	GLU
2	D	118	LEU
2	D	143	ARG
2	D	147	THR
2	D	160	ILE
2	D	183	ASP
2	D	192	ILE
2	D	212	ILE
2	D	236	TRP
2	D	268	THR
2	D	280	SER
2	D	289	ARG
2	D	325	ILE
2	D	333	PHE
2	D	341	GLU
2	D	349	ASN
2	D	357	MET
2	D	362	THR
2	D	368	ASP
2	D	375	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	93	ASN
1	A	120	GLN
1	A	133	ASN
1	A	157	ASN
1	A	253	GLN
1	A	267	GLN
1	A	274	GLN
1	A	279	ASN
1	A	283	GLN
1	A	319	GLN
1	A	399	HIS
1	A	409	GLN
1	A	443	ASN
1	A	447	ASN
1	A	457	ASN
1	A	472	HIS
1	A	473	GLN
1	A	493	ASN
1	A	526	GLN
1	A	564	GLN
2	D	11	ASN
2	D	48	ASN
2	D	71	GLN
2	D	117	ASN
2	D	154	ASN
2	D	168	ASN
2	D	205	ASN
2	D	241	ASN
2	D	256	HIS
2	D	273	ASN
2	D	299	GLN
2	D	315	ASN
2	D	317	ASN
2	D	349	ASN
2	D	354	HIS
2	D	374	ASN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	PO4	A	586	-	0,2,4	-	-	0,1,6	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	586	PO4	0	1

5.7 Other polymers [i](#)

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	571/584 (97%)	0.08	28 (4%) 35 27	10, 44, 94, 126	0
2	D	361/391 (92%)	0.44	26 (7%) 21 16	18, 53, 95, 109	0
All	All	932/975 (95%)	0.22	54 (5%) 29 22	10, 49, 95, 126	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	217	SER	5.5
2	D	367	ILE	5.2
1	A	566	THR	4.2
2	D	368	ASP	4.2
1	A	349	SER	4.0
1	A	576	SER	3.9
1	A	555	ALA	3.5
2	D	364	LEU	3.4
1	A	572	ILE	3.3
2	D	347	SER	3.2
1	A	352	ALA	3.2
1	A	575	GLY	3.0
1	A	574	ILE	3.0
1	A	542	VAL	2.9
2	D	55	TYR	2.8
2	D	334	LYS	2.8
2	D	361	ALA	2.8
2	D	60	ILE	2.8
1	A	350	LEU	2.8
2	D	214	GLY	2.7
1	A	559	SER	2.7
1	A	356	THR	2.7
1	A	567	ILE	2.6
2	D	376	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	573	ASP	2.6
2	D	244	LYS	2.5
2	D	366	THR	2.5
2	D	61	HIS	2.5
2	D	105	ILE	2.5
1	A	331	ILE	2.4
1	A	284	MET	2.4
2	D	216	PRO	2.4
1	A	568	ASP	2.3
2	D	202	MET	2.3
2	D	57	SER	2.3
1	A	449	LEU	2.3
1	A	536	TRP	2.3
1	A	565	TYR	2.2
1	A	347	ALA	2.2
1	A	355	ALA	2.2
2	D	243	HIS	2.2
2	D	77	ALA	2.2
2	D	226	LEU	2.2
2	D	377	LYS	2.1
1	A	360	SER	2.1
1	A	252	MET	2.1
2	D	54	PHE	2.1
1	A	280	MET	2.1
2	D	96	SER	2.0
1	A	267	GLN	2.0
2	D	363	LYS	2.0
1	A	346	PRO	2.0
1	A	353	MET	2.0
2	D	11	ASN	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(Å ²)	Q<0.9
3	K	A	585	1/1	0.88	0.12	46,46,46,46	1
4	PO4	A	586	3/5	0.96	0.11	28,28,29,99	2

6.5 Other polymers [i](#)

There are no such residues in this entry.