



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WTH  
Title : Crystal structure of gp5-S351L mutant and gp27 complex  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

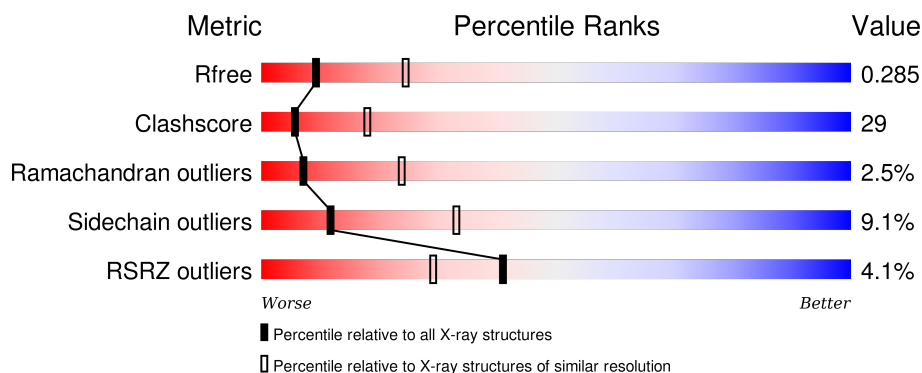
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>4%</div> <div>58%</div> <div>33%</div> <div>6%</div> <div>.</div> </div>
2	D	391	<div> <div>4%</div> <div>46%</div> <div>39%</div> <div>7%</div> <div>.</div> <div>8%</div> </div>

## 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	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 (three-letter code: K) (formula: K).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

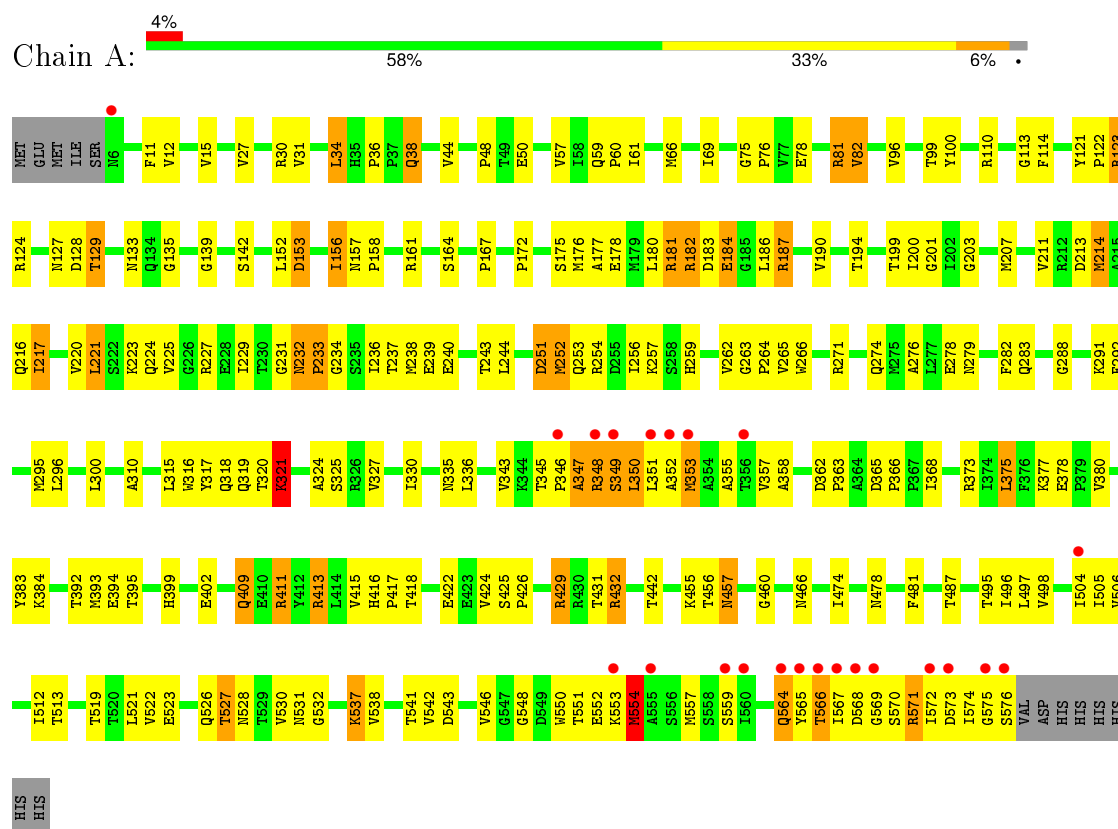
- Molecule 5 is water.

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

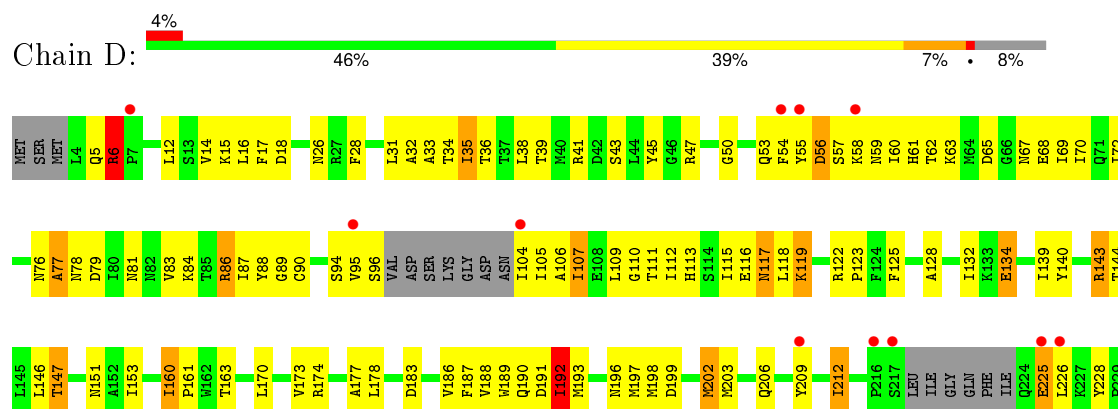
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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: Tail-associated lysozyme



#### • Molecule 2: Baseplate structural protein Gp27



F326	L230
R327	
D328	F234
S329	Y235
K330	H236
R331	
Q332	S240
F333	N241
K334	
F337	R245
Y338	D246
Y339	P247
D340	N248
E341	K249
V342	N250
I343	
H344	Y254
E345	
L346	D260
S347	
N348	T268
N349	
N350	E272
S351	N273
V352	S274
T353	
H354	R279
L355	S280
Y356	Q281
M357	Y283
	S284
T362	E285
K363	N286
T366	T287
I367	Y288
D368	R289
F369	N290
V370	
K371	E293
E375	I296
F376	R297
K377	
SER	Q303
ASP	
THR	A308
THR	
THR	G314
GLU	N315
SER	F316
SER	N317
SER	L318
SER	T319
SER	P320
SER	Q321
ASN	Y322
LYS	K323
GLN	I324
	I325

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (11.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 35805 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	A	0.41	1/4479 (0.0%)	0.64	1/6074 (0.0%)
2	D	0.45	1/2964 (0.0%)	0.68	4/4018 (0.1%)
All	All	0.43	2/7443 (0.0%)	0.65	5/10092 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	192	ILE	C-O	-6.04	1.11	1.23
1	A	554	MET	C-N	-5.02	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	MET	CB-CA-C	-6.45	97.49	110.40
2	D	192	ILE	CA-C-N	-6.05	103.89	117.20
2	D	151	ASN	CB-CA-C	5.33	121.07	110.40
2	D	368	ASP	CB-CA-C	5.31	121.01	110.40
1	A	432	ARG	CB-CA-C	5.30	121.01	110.40

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	4309	257	0
2	D	2897	0	2828	166	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	7137	421	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 29.

All (421) 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: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
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
2:D:117:ASN:O	2:D:119:LYS:HD2	1.86	0.75
1:A:384:LYS:CB	1:A:409:GLN:HG2	2.18	0.73
1:A:214:MET:HE1	1:A:217:ILE:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:HA	1:A:223:LYS:HE2	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
1:A:50:GLU:CD	1:A:50:GLU:H	1.94	0.70
1:A:571:ARG:C	1:A:572:ILE:HD12	2.11	0.69
2:D:144:THR:O	2:D:147:THR:HG23	1.92	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
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:366:THR:O	2:D:368:ASP:N	2.28	0.67
1:A:190:VAL:HG21	1:A:214:MET:HE1	1.77	0.66
2:D:349:ASN:ND2	2:D:350:ASN:N	2.38	0.66
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: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
1:A:552:GLU:HB2	1:A:554:MET:HE1	1.79	0.64
2:D:140:TYR:CB	2:D:147:THR:HG22	2.26	0.64
2:D:347:SER:HB3	2:D:349:ASN:ND2	2.12	0.64
1:A:232:ASN:HB3	1:A:233:PRO:HD3	1.77	0.64
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
2:D:366:THR:O	2:D:369:PRO:HD3	1.98	0.63
1:A:530:VAL:C	1:A:532:GLY:H	2.01	0.63
1:A:221:LEU:HB3	1:A:229:ILE:HD12	1.80	0.63
1:A:522:VAL:HG23	1:A:522:VAL:O	1.99	0.63
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:176:MET:HG3	1:A:278:GLU:OE2	1.99	0.62
2:D:31:LEU:C	2:D:33:ALA:H	2.03	0.62
1:A:177:ALA:O	1:A:181:ARG:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:ILE:HG21	2:D:202:MET:HE3	1.81	0.62
1:A:574:ILE:N	1:A:574:ILE:HD12	2.14	0.61
1:A:573:ASP:C	1:A:574:ILE:HD12	2.20	0.61
2:D:86:ARG:HH11	2:D:192:ILE:HB	1.66	0.61
1:A:152:LEU:HD22	1:A:378:GLU:HG2	1.81	0.61
2:D:86:ARG:HG3	2:D:87:ILE:N	2.13	0.61
1:A:44:VAL:O	2:D:122:ARG:HG2	2.01	0.61
1:A:564:GLN:HE21	1:A:564:GLN:HA	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:495:THR:C	1:A:496:ILE:HD12	2.22	0.60
1:A:541:THR:O	1:A:542:VAL:CG2	2.47	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:350:LEU:HB3	1:A:355:ALA:CB	2.31	0.60
1:A:213:ASP:O	1:A:217:ILE:HG12	2.02	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:O	2:D:35:ILE:HD13	2.02	0.60
2:D:250:ASN:HD21	2:D:272:GLU:HB2	1.67	0.60
2:D:367:ILE:O	2:D:367:ILE:HG22	2.02	0.60
2:D:314:GLY:HA3	2:D:351:SER:OG	2.01	0.60
1:A:416:HIS:CE1	1:A:418:THR:HG23	2.37	0.59
2:D:349:ASN:HD22	2:D:349:ASN:H	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
2:D:143:ARG:HB3	2:D:146:LEU:HD12	1.85	0.59
1:A:330:ILE:HD13	1:A:335:ASN:O	2.03	0.59
1:A:200:ILE:HG12	1:A:201:GLY:H	1.67	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
1:A:237:THR:HG22	1:A:240:GLU:CB	2.30	0.58
1:A:176:MET:O	1:A:180:LEU:HB2	2.04	0.58
1:A:152:LEU:HD11	1:A:380:VAL:HG12	1.84	0.58
2:D:104:ILE:O	2:D:104:ILE:HG23	2.04	0.58
2:D:160:ILE:H	2:D:160:ILE:HD13	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASP:OD2	1:A:216:GLN:HG3	2.04	0.58
1:A:552:GLU:HB2	1:A:554:MET:HE2	1.86	0.57
1:A:61:ILE:HD12	1:A:61:ILE:C	2.25	0.57
1:A:424:VAL:HA	1:A:429:ARG:O	2.04	0.57
2:D:290:ASN:ND2	2:D:371:LYS:HA	2.14	0.57
2:D:119:LYS:HG3	5:D:530:HOH:O	2.04	0.57
1:A:569:GLY:C	1:A:571:ARG:H	2.06	0.57
1:A:48:PRO:HB2	1:A:50:GLU:OE2	2.04	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:NE2	1:A:564:GLN:HA	2.20	0.57
2:D:56:ASP:OD1	2:D:57:SER:N	2.37	0.57
1:A:12:VAL:CG1	1:A:100:TYR:OH	2.53	0.57
1:A:257:LYS:HE3	1:A:266:TRP:CH2	2.40	0.57
2:D:5:GLN:HG3	5:D:499:HOH:O	2.06	0.56
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
1:A:157:ASN:HD22	1:A:158:PRO:CD	2.14	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
1:A:12:VAL:HG11	1:A:100:TYR:OH	2.05	0.56
1:A:237:THR:HG22	1:A:240:GLU:CD	2.26	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
1:A:552:GLU:C	1:A:554:MET:HE1	2.26	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:526:GLN:HG2	1:A:527:THR:N	2.22	0.55
1:A:276:ALA:HB2	1:A:330:ILE:HG21	1.88	0.55
1:A:186:LEU:O	1:A:187:ARG:HD2	2.07	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
2:D:212:ILE:HD13	2:D:230:LEU:HA	1.89	0.54
2:D:58:LYS:HB3	2:D:58:LYS:NZ	2.22	0.54
2:D:283:TYR:O	2:D:286:MET:HG2	2.07	0.54
1:A:526:GLN:C	1:A:527:THR:HG22	2.27	0.54
2:D:132:ILE:HD12	2:D:197:MET:HE1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:456:THR:HG22	1:A:457:ASN:N	2.23	0.54
2:D:212:ILE:HG13	2:D:226:LEU:HD22	1.90	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: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
1:A:496:ILE:HG22	1:A:497:LEU:N	2.23	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:186:LEU:C	1:A:187:ARG:HD2	2.29	0.53
1:A:368:ILE:HD12	1:A:368:ILE:N	2.22	0.53
2:D:193:MET:HA	2:D:193:MET:HE2	1.91	0.53
1:A:164:SER:HB3	5:A:636:HOH:O	2.08	0.53
2:D:349:ASN:HD22	2:D:349:ASN:N	2.04	0.53
1:A:357:VAL:O	1:A:357:VAL:HG12	2.08	0.53
1:A:236:ILE:HG13	1:A:240:GLU:HB3	1.91	0.53
1:A:474:ILE:HD11	1:A:478:ASN:HB2	1.91	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:365:ASP:HB3	1:A:366:PRO:HD2	1.90	0.53
1:A:318:GLN:O	1:A:321:LYS:HD2	2.09	0.52
2:D:35:ILE:C	2:D:35:ILE:HD13	2.29	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
1:A:319:GLN:HG3	5:A:651:HOH:O	2.07	0.52
2:D:95:VAL:HG13	2:D:105:ILE:HG22	1.91	0.52
2:D:18:ASP:HA	2:D:68:GLU:HG3	1.90	0.52
2:D:189:TRP:CD1	2:D:320:PRO:HG2	2.45	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:353:MET:O	1:A:357:VAL:HG23	2.09	0.52
1:A:321:LYS:HB2	1:A:460:GLY:HA2	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG13	1:A:27:VAL:HB	1.92	0.51
1:A:133:ASN:HD21	1:A:392:THR:N	1.97	0.51
1:A:512:ILE:N	1:A:512:ILE:CD1	2.71	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
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: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
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:557:MET:CE	1:A:559:SER:HB2	2.41	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:157:ASN:ND2	1:A:158:PRO:HD2	2.12	0.50
2:D:225:GLU:HG3	2:D:225:GLU:O	2.11	0.50
1:A:392:THR:HG23	1:A:402:GLU:HG2	1.93	0.50
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:207:MET:SD	1:A:211:VAL:HG21	2.52	0.50
1:A:350:LEU:HD23	1:A:350:LEU:N	2.21	0.50
1:A:200:ILE:HG12	1:A:201:GLY:N	2.26	0.50
1:A:504:ILE:O	1:A:505:ILE:HD13	2.12	0.50
1:A:57:VAL:HG12	1:A:96:VAL:HB	1.93	0.50
2:D:140:TYR:CD1	2:D:143:ARG:NH2	2.79	0.49
2:D:283:TYR:C	2:D:285:GLU:H	2.15	0.49
2:D:43:SER:HA	2:D:341:GLU:HB2	1.94	0.49
2:D:107:ILE:CD1	2:D:109:LEU:HD12	2.42	0.49
2:D:53:GLN:HB3	2:D:106:ALA:CB	2.40	0.49
2:D:241:ASN:HD22	2:D:241:ASN:C	2.15	0.49
1:A:512:ILE:HD12	1:A:512:ILE:H	1.74	0.49
2:D:53:GLN:HA	2:D:106:ALA:HA	1.93	0.49
2:D:349:ASN:CG	2:D:350:ASN:H	2.14	0.49
2:D:56:ASP:OD2	2:D:60:ILE:HG22	2.12	0.49
2:D:186:VAL:HG12	2:D:187:PHE:N	2.26	0.49
1:A:135:GLY:HA2	1:A:383:TYR:OH	2.13	0.49
2:D:6:ARG:HD2	2:D:6:ARG:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CD1	1:A:11:PHE:C	2.86	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:496:ILE:CG2	1:A:497:LEU:N	2.76	0.48
1:A:256:ILE:HG23	1:A:257:LYS:N	2.28	0.48
2:D:325:ILE:HD13	2:D:326:PHE:N	2.28	0.48
2:D:41:ARG:HG3	2:D:343:ILE:CG1	2.38	0.48
1:A:324:ALA:HA	1:A:327:VAL:HG22	1.94	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:214:MET:HE1	1:A:217:ILE:CG2	2.40	0.48
1:A:474:ILE:CD1	1:A:478:ASN:HB2	2.44	0.48
2:D:77:ALA:O	2:D:78:ASN:C	2.52	0.48
1:A:546:VAL:HG22	1:A:548:GLY:H	1.78	0.48
1:A:429:ARG:HH11	1:A:431:THR:CB	2.26	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:84:LYS:HG2	2:D:193:MET:HE1	1.96	0.47
2:D:303:GLN:OE1	2:D:363:LYS:HD2	2.14	0.47
1:A:199:THR:HG22	1:A:200:ILE:N	2.29	0.47
1:A:81:ARG:NH2	1:A:128:ASP:OD1	2.45	0.47
1:A:127:ASN:CG	1:A:129:THR:HG23	2.35	0.47
2:D:190:GLN:HG3	5:D:536:HOH:O	2.15	0.47
1:A:175:SER:HB3	1:A:178:GLU:HG3	1.96	0.47
1:A:362:ASP:OD1	1:A:363:PRO:HD2	2.14	0.47
1:A:512:ILE:CD1	1:A:512:ILE:H	2.27	0.47
2:D:338:TYR:O	2:D:357:MET:HB2	2.14	0.47
1:A:225:VAL:HG11	1:A:236:ILE:HD11	1.96	0.47
1:A:214:MET:HE2	1:A:234:GLY:H	1.80	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
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
1:A:541:THR:C	1:A:542:VAL:HG23	2.35	0.47
2:D:345:GLU:HB3	2:D:352:VAL:CG2	2.45	0.47
1:A:167:PRO:CG	1:A:343:VAL:HG11	2.44	0.47
1:A:66:MET:O	1:A:69:ILE:HG12	2.15	0.47
1:A:239:GLU:CD	1:A:239:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ARG:HA	1:A:373:ARG:HE	1.80	0.46
1:A:512:ILE:HG22	1:A:513:THR:N	2.29	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:568:ASP:CG	1:A:569:GLY:H	2.18	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
2:D:199:ASP:OD2	2:D:202:MET:HG3	2.15	0.46
1:A:429:ARG:HH11	1:A:431:THR:HB	1.79	0.46
2:D:268:THR:O	2:D:268:THR:HG22	2.14	0.46
1:A:526:GLN:NE2	1:A:528:ASN:HD21	2.14	0.46
1:A:252:MET:HE3	1:A:278:GLU:HA	1.98	0.46
2:D:325:ILE:C	2:D:325:ILE:HD13	2.35	0.46
1:A:156:ILE:C	1:A:156:ILE:HD12	2.36	0.46
1:A:349:SER:HB2	1:A:350:LEU:HD23	1.97	0.46
1:A:237:THR:CG2	1:A:240:GLU:HB2	2.39	0.46
1:A:564:GLN:CA	1:A:564:GLN:HE21	2.26	0.46
1:A:184:GLU:CG	1:A:203:GLY:CA	2.85	0.46
1:A:346:PRO:C	1:A:348:ARG:H	2.20	0.46
2:D:212:ILE:HD12	2:D:228:TYR:O	2.16	0.46
2:D:112:ILE:HG22	2:D:113:HIS:N	2.31	0.46
2:D:325:ILE:O	2:D:325:ILE:HG23	2.16	0.46
1:A:227:ARG:HG2	5:A:770:HOH:O	2.14	0.45
1:A:223:LYS:HE3	5:A:661:HOH:O	2.16	0.45
1:A:220:VAL:O	1:A:224:GLN:HG3	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
1:A:572:ILE:N	1:A:572:ILE:HD12	2.31	0.45
2:D:212:ILE:CD1	2:D:230:LEU:HA	2.45	0.45
2:D:107:ILE:HD13	2:D:107:ILE:C	2.37	0.45
2:D:160:ILE:HG21	2:D:282:ALA:HB1	1.98	0.45
2:D:212:ILE:HD11	2:D:226:LEU:HD13	1.98	0.45
2:D:206:GLN:OE1	2:D:322:VAL:HA	2.16	0.45
1:A:59:GLN:HB3	1:A:60:PRO:HD2	1.97	0.45
1:A:265:VAL:HA	1:A:300:LEU:HD21	1.98	0.45
2:D:43:SER:HB3	2:D:47:ARG:HB3	1.99	0.45
2:D:375:GLU:H	2:D:375:GLU:CD	2.20	0.45
1:A:243:THR:O	1:A:244:LEU:C	2.55	0.45
2:D:178:LEU:C	2:D:178:LEU:HD13	2.37	0.45
2:D:72:ILE:HD12	2:D:88:TYR:CE1	2.52	0.45
1:A:182:ARG:HG3	1:A:183:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:VAL:C	1:A:532:GLY:N	2.66	0.45
2:D:31:LEU:C	2:D:33:ALA:N	2.69	0.45
2:D:95:VAL:HG22	2:D:105:ILE:HG21	1.99	0.44
2:D:16:LEU:HD12	2:D:16:LEU:C	2.37	0.44
2:D:245:ARG:HD2	5:D:478:HOH:O	2.17	0.44
2:D:330:LYS:HG3	2:D:330:LYS:O	2.17	0.44
1:A:251:ASP:O	1:A:254:ARG:HG2	2.16	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
2:D:283:TYR:C	2:D:285:GLU:N	2.71	0.44
2:D:319:THR:O	2:D:322:VAL:HG13	2.18	0.44
2:D:367:ILE:CG2	2:D:367:ILE:O	2.65	0.44
1:A:30:ARG:NH2	1:A:30:ARG:HG3	2.33	0.44
2:D:250:ASN:ND2	2:D:272:GLU:HB2	2.33	0.44
1:A:161:ARG:NH1	1:A:167:PRO:HD2	2.32	0.44
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.81	0.44
1:A:81:ARG:HG2	5:A:609:HOH:O	2.17	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:541:THR:CG2	1:A:542:VAL:H	2.14	0.44
2:D:375:GLU:N	2:D:375:GLU:CD	2.71	0.44
1:A:348:ARG:HD3	1:A:349:SER:H	1.82	0.43
1:A:82:VAL:HG23	1:A:99:THR:HG22	2.00	0.43
1:A:352:ALA:O	1:A:353:MET:HB2	2.18	0.43
2:D:12:LEU:HD11	2:D:14:VAL:CG2	2.48	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: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
2:D:79:ASP:C	2:D:81:ASN:N	2.71	0.43
1:A:184:GLU:HG3	1:A:203:GLY:CA	2.47	0.43
1:A:393:MET:HG2	1:A:394:GLU:N	2.32	0.43
2:D:332:GLN:HG2	2:D:332:GLN:O	2.19	0.43
2:D:111:THR:O	2:D:115:ILE:HG12	2.18	0.43
1:A:263:GLY:N	1:A:264:PRO:HD2	2.34	0.43
1:A:425:SER:OG	1:A:429:ARG:HB3	2.18	0.43
1:A:121:TYR:HA	1:A:122:PRO:C	2.39	0.43
1:A:416:HIS:CG	1:A:417:PRO:HD2	2.53	0.43
2:D:240:SER:CB	2:D:245:ARG:HH12	2.29	0.42
1:A:315:LEU:O	1:A:319:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:C	1:A:347:ALA:H	2.22	0.42
1:A:236:ILE:HA	1:A:236:ILE:HD12	1.92	0.42
2:D:107:ILE:HD12	2:D:109:LEU:HD12	2.01	0.42
2:D:349:ASN:HD22	2:D:350:ASN:N	2.15	0.42
1:A:350:LEU:CD2	1:A:350:LEU:H	2.23	0.42
1:A:81:ARG:HB3	1:A:100:TYR:CZ	2.55	0.42
2:D:315:ASN:C	2:D:315:ASN:ND2	2.72	0.42
1:A:348:ARG:HG2	1:A:349:SER:N	2.35	0.42
2:D:6:ARG:HD2	2:D:6:ARG:H	1.84	0.42
1:A:526:GLN:HE21	1:A:528:ASN:HD21	1.67	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
2:D:349:ASN:CG	2:D:350:ASN:N	2.72	0.42
2:D:189:TRP:CE2	2:D:196:ASN:HB2	2.55	0.42
2:D:186:VAL:CG1	2:D:187:PHE:N	2.83	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:481:PHE:C	1:A:481:PHE:CD1	2.93	0.42
1:A:566:THR:OG1	1:A:567:ILE:N	2.53	0.41
1:A:422:GLU:HA	1:A:431:THR:O	2.20	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:474:ILE:HD11	1:A:478:ASN:N	2.36	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:75:GLY:N	1:A:76:PRO:HD2	2.35	0.41
1:A:557:MET:HE2	1:A:559:SER:HB2	2.02	0.41
2:D:234:PHE:HE1	2:D:326:PHE:CE1	2.38	0.41
1:A:552:GLU:C	1:A:553:LYS:HD2	2.40	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:353:THR:HG22	2:D:355:LEU:CD1	2.50	0.41
2:D:39:THR:O	2:D:50:GLY:CA	2.68	0.41
1:A:110:ARG:NH2	5:A:766:HOH:O	2.53	0.41
1:A:320:THR:O	1:A:320:THR:HG22	2.21	0.41
2:D:346:LEU:HD12	2:D:346:LEU:O	2.21	0.41
1:A:186:LEU:HD21	1:A:238:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:LYS:HE3	2:D:193:MET:SD	2.61	0.41
1:A:207:MET:CE	1:A:220:VAL:HG21	2.51	0.41
2:D:297:ARG:HD3	5:D:419:HOH:O	2.20	0.41
2:D:288:TYR:CE2	2:D:371:LYS:HD2	2.56	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
1:A:153:ASP:O	1:A:377:LYS:HG3	2.21	0.41
1:A:569:GLY:C	1:A:571:ARG:N	2.73	0.40
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:333:PHE:CD1	2:D:333:PHE:N	2.89	0.40
2:D:293:GLU:HA	2:D:296:ILE:HG22	2.02	0.40
1:A:553:LYS:N	1:A:554:MET:HE1	2.36	0.40
1:A:30:ARG:HH21	1:A:30:ARG:HG3	1.85	0.40
1:A:239:GLU:O	1:A:240:GLU:C	2.60	0.40
2:D:160:ILE:HG21	2:D:282:ALA:CB	2.52	0.40
1:A:30:ARG:NE	1:A:113:GLY:HA3	2.35	0.40
2:D:328:ASP:CG	2:D:329:SER:H	2.25	0.40
2:D:346:LEU:HD12	2:D:346:LEU:C	2.41	0.40
1:A:557:MET:HE1	1:A:559:SER:HB2	2.04	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:249:LYS:O	2:D:268:THR:HG23	2.21	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%)	7	24
2	D	355/391 (91%)	300 (84%)	46 (13%)	9 (2%)	7	24
All	All	924/975 (95%)	783 (85%)	118 (13%)	23 (2%)	7	24

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%)	440 (92%)	41 (8%)	13	36
2	D	322/350 (92%)	290 (90%)	32 (10%)	10	28
All	All	803/844 (95%)	730 (91%)	73 (9%)	12	33

All (73) 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	81	ARG
1	A	82	VAL
1	A	123	ARG
1	A	129	THR
1	A	153	ASP
1	A	156	ILE
1	A	181	ARG
1	A	182	ARG
1	A	184	GLU
1	A	187	ARG
1	A	194	THR
1	A	214	MET
1	A	221	LEU
1	A	251	ASP
1	A	252	MET
1	A	271	ARG
1	A	279	ASN
1	A	321	LYS
1	A	348	ARG
1	A	350	LEU
1	A	353	MET
1	A	375	LEU
1	A	409	GLN
1	A	411	ARG
1	A	413	ARG
1	A	429	ARG
1	A	432	ARG
1	A	442	THR
1	A	457	ASN
1	A	466	ASN
1	A	487	THR
1	A	498	VAL

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Mol	Chain	Res	Type
1	A	506	VAL
1	A	523	GLU
1	A	527	THR
1	A	537	LYS
1	A	554	MET
1	A	566	THR
2	D	6	ARG
2	D	35	ILE
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	116	GLU
2	D	118	LEU
2	D	119	LYS
2	D	134	GLU
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	241	ASN
2	D	268	THR
2	D	280	SER
2	D	289	ARG
2	D	315	ASN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	59	GLN
1	A	93	ASN
1	A	120	GLN
1	A	133	ASN
1	A	157	ASN
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	443	ASN
1	A	457	ASN
1	A	473	GLN
1	A	493	ASN
1	A	526	GLN
1	A	528	ASN
1	A	533	ASN
1	A	564	GLN
2	D	48	ASN
2	D	71	GLN
2	D	117	ASN
2	D	151	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	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 carbohydrates 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	0.00	-	0,1,6	0.00	-

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	PO4	A	586	-	-	0/0/0/0	0/0/0/0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	571/584 (97%)	0.14	23 (4%) 42 30	10, 44, 94, 126	0
2	D	361/391 (92%)	0.16	15 (4%) 40 28	18, 53, 95, 109	0
All	All	932/975 (95%)	0.15	38 (4%) 41 29	10, 49, 95, 126	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	SER	9.2
2	D	217	SER	5.9
1	A	576	SER	5.2
1	A	572	ILE	4.8
1	A	352	ALA	4.2
1	A	353	MET	4.2
1	A	568	ASP	4.0
2	D	367	ILE	3.9
1	A	566	THR	3.9
1	A	351	LEU	3.7
1	A	555	ALA	3.6
2	D	216	PRO	3.5
2	D	55	TYR	3.4
2	D	376	PHE	3.2
2	D	95	VAL	3.2
2	D	226	LEU	3.2
2	D	368	ASP	2.8
1	A	565	TYR	2.8
1	A	575	GLY	2.6
1	A	569	GLY	2.5
2	D	209	TYR	2.5
1	A	573	ASP	2.4
1	A	504	ILE	2.3
1	A	346	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	225	GLU	2.3
2	D	54	PHE	2.3
1	A	567	ILE	2.3
1	A	560	ILE	2.2
1	A	6	ASN	2.1
2	D	328	ASP	2.1
1	A	559	SER	2.1
2	D	58	LYS	2.1
1	A	564	GLN	2.1
1	A	356	THR	2.1
1	A	553	LYS	2.1
2	D	104	ILE	2.0
1	A	348	ARG	2.0
2	D	7	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	A	586	3/5	0.94	0.16	-	28,28,29,99	2
3	K	A	585	1/1	0.94	0.19	-	46,46,46,46	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.