



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 05:14 AM EDT

PDB ID : 2Z6B
Title : Crystal Structure Analysis of (gp27-gp5)3 conjugated with Fe(III) protoporphyrin
Authors : Koshiyama, T.; Yokoi, N.; Ueno, T.; Kanamaru, S.; Nagano, S.; Shiro, Y.; Arisaka, F.; Watanabe, Y.
Deposited on : 2007-07-28
Resolution : 3.11 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

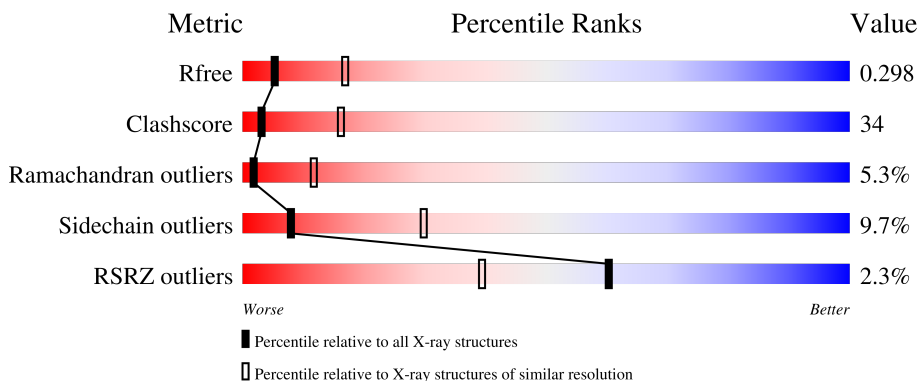
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	<div> <div></div> <div>55%</div> <div>37%</div> <div>6%</div> </div>
2	D	391	<div> <div>4%</div> <div>39%</div> <div>44%</div> <div>11%</div> <div>6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7389 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	573	Total	C	N	O	S	0	0	0
			4273	2645	744	862	22			

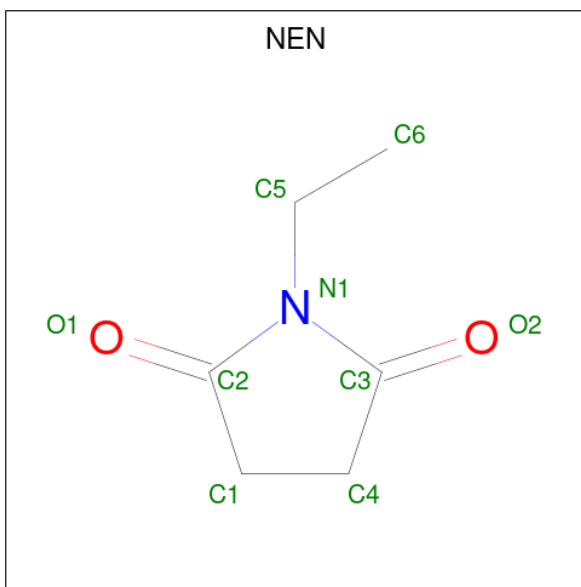
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	CYS	ASN	engineered mutation	UNP P16009
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	368	Total	C	N	O	S	0	0	0
			2786	1779	453	537	17			

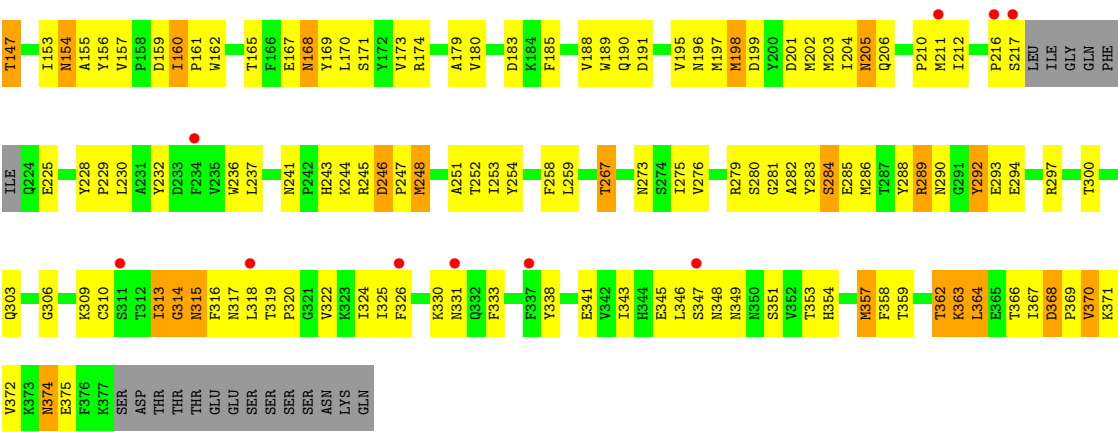
- Molecule 3 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (three-letter code: NEN) (formula: $C_6H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	D	133	Total	O	0	0
			133	133		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.54Å 138.54Å 389.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.64 – 3.11 45.04 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.64-3.11) 97.7 (45.04-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.36 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.315 0.225 , 0.298	Depositor DCC
R_{free} test set	1287 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7389	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.39	0/4355	0.67	0/5931
2	D	0.35	0/2853	0.60	0/3894
All	All	0.37	0/7208	0.64	0/9825

There are no bond length outliers.

There are no bond angle outliers.

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	4273	0	4022	248	0
2	D	2786	0	2542	218	0
3	A	9	0	7	0	0
4	A	188	0	0	4	0
4	D	133	0	0	1	0
All	All	7389	0	6571	458	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 34.

All (458) 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:97:VAL:HG12	2:D:98:ASP:H	1.05	1.10
1:A:38:GLN:H	1:A:38:GLN:NE2	1.56	1.04
2:D:313:ILE:HD12	2:D:313:ILE:H	1.28	0.97
1:A:375:LEU:HD22	1:A:455:LYS:HG2	1.46	0.94
1:A:232:ASN:HB3	1:A:233:PRO:HD3	1.50	0.93
1:A:36:PRO:HB2	1:A:38:GLN:HE22	1.32	0.93
2:D:90:CYS:HB2	2:D:107:ILE:HD11	1.52	0.91
1:A:200:ILE:HG12	1:A:201:GLY:H	1.36	0.89
2:D:199:ASP:H	2:D:202:MET:HE3	1.35	0.89
2:D:97:VAL:HG12	2:D:98:ASP:N	1.87	0.89
1:A:36:PRO:HB2	1:A:38:GLN:NE2	1.88	0.88
1:A:184:GLU:HG2	1:A:203:GLY:HA3	1.54	0.87
1:A:237:THR:HB	1:A:240:GLU:HG3	1.55	0.87
2:D:237:LEU:HD22	2:D:237:LEU:H	1.39	0.86
1:A:31:VAL:HB	1:A:34:LEU:HD11	1.58	0.85
1:A:18:ARG:NH1	1:A:77:VAL:HA	1.89	0.85
1:A:156:ILE:H	1:A:457:ASN:HD21	1.19	0.85
2:D:97:VAL:CG1	2:D:98:ASP:H	1.90	0.84
1:A:237:THR:HG22	1:A:238:MET:H	1.43	0.83
1:A:394:GLU:HG3	1:A:400:ILE:HG12	1.61	0.82
1:A:384:LYS:HB2	1:A:409:GLN:HG2	1.64	0.80
1:A:392:THR:OG1	1:A:402:GLU:HB3	1.82	0.79
1:A:373:ARG:HA	1:A:373:ARG:HE	1.48	0.79
1:A:18:ARG:HH12	1:A:77:VAL:HG12	1.47	0.79
1:A:18:ARG:HH11	1:A:77:VAL:HA	1.44	0.78
2:D:53:GLN:HA	2:D:105:ILE:O	1.82	0.78
1:A:48:PRO:HD2	1:A:51:LYS:HG3	1.66	0.78
1:A:196:GLY:O	1:A:210:PRO:HA	1.84	0.78
1:A:127:ASN:OD1	1:A:129:THR:HG23	1.84	0.78
1:A:176:MET:HE1	1:A:278:GLU:HB2	1.66	0.78
2:D:135:MET:O	2:D:139:ILE:HG12	1.84	0.77
2:D:318:LEU:HD12	2:D:353:THR:HG21	1.67	0.77
1:A:220:VAL:O	1:A:224:GLN:HG3	1.85	0.76
1:A:323:ARG:HA	1:A:326:ARG:HH21	1.50	0.76
2:D:201:ASP:O	2:D:204:ILE:HG22	1.84	0.76
1:A:214:MET:HE2	1:A:232:ASN:O	1.86	0.76
1:A:31:VAL:HB	1:A:34:LEU:CD1	2.16	0.75
2:D:23:TRP:HE1	2:D:71:GLN:HE22	1.32	0.75
1:A:17:ASP:HB3	1:A:28:ARG:HD2	1.68	0.75
2:D:366:THR:O	2:D:368:ASP:N	2.20	0.75
1:A:147:ILE:HD13	1:A:186:LEU:HD23	1.68	0.75
2:D:117:ASN:ND2	2:D:165:THR:HG21	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:LEU:HD13	2:D:52:LEU:HD13	1.69	0.74
1:A:38:GLN:H	1:A:38:GLN:CD	1.91	0.74
1:A:416:HIS:HE1	1:A:418:THR:HG23	1.53	0.74
2:D:112:ILE:O	2:D:116:GLU:HG3	1.87	0.74
1:A:237:THR:HG22	1:A:238:MET:N	2.02	0.73
1:A:335:ASN:C	1:A:335:ASN:HD22	1.92	0.73
1:A:38:GLN:NE2	1:A:38:GLN:N	2.34	0.73
1:A:133:ASN:HD21	1:A:392:THR:H	1.37	0.73
1:A:50:GLU:CD	1:A:50:GLU:H	1.93	0.72
2:D:48:ASN:OD1	2:D:190:GLN:HB2	1.90	0.72
2:D:132:ILE:HD12	2:D:197:MET:HE1	1.72	0.72
2:D:363:LYS:HG2	2:D:364:LEU:H	1.55	0.71
2:D:23:TRP:HE1	2:D:71:GLN:NE2	1.88	0.71
2:D:56:ASP:CG	2:D:60:ILE:H	1.95	0.70
2:D:125:PHE:HE1	2:D:134:GLU:HG3	1.56	0.70
1:A:199:THR:HG22	1:A:200:ILE:N	2.07	0.70
2:D:313:ILE:HD12	2:D:313:ILE:N	2.03	0.70
1:A:39:ARG:HH22	1:A:112:GLU:C	1.94	0.69
2:D:128:ALA:O	2:D:132:ILE:HG13	1.93	0.69
2:D:363:LYS:CG	2:D:364:LEU:H	2.06	0.69
2:D:313:ILE:H	2:D:313:ILE:CD1	2.05	0.69
1:A:390:VAL:HG22	1:A:404:ASP:OD1	1.94	0.68
1:A:184:GLU:CG	1:A:203:GLY:HA3	2.22	0.68
2:D:86:ARG:HG2	2:D:86:ARG:HH21	1.58	0.68
1:A:214:MET:HE1	1:A:234:GLY:H	1.58	0.68
2:D:20:TYR:CZ	2:D:143:ARG:HA	2.29	0.67
2:D:111:THR:HB	2:D:113:HIS:CE1	2.30	0.67
2:D:56:ASP:OD1	2:D:60:ILE:HG12	1.95	0.67
1:A:410:GLU:CD	1:A:410:GLU:H	1.99	0.66
1:A:156:ILE:H	1:A:457:ASN:ND2	1.92	0.66
1:A:375:LEU:HD13	1:A:455:LYS:HB3	1.77	0.66
1:A:183:ASP:HB3	1:A:323:ARG:NE	2.11	0.65
2:D:237:LEU:H	2:D:237:LEU:CD2	2.09	0.65
1:A:57:VAL:HG11	4:A:622:HOH:O	1.96	0.65
1:A:90:TRP:CH2	2:D:171:SER:HB2	2.32	0.65
2:D:16:LEU:HD13	2:D:16:LEU:O	1.96	0.65
1:A:316:TRP:HH2	1:A:327:VAL:CG2	2.10	0.64
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.62	0.64
2:D:118:LEU:HD22	2:D:119:LYS:H	1.63	0.64
1:A:48:PRO:HB2	1:A:50:GLU:OE1	1.98	0.64
1:A:554:MET:HG3	1:A:556:SER:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:CD	1:A:50:GLU:N	2.50	0.63
2:D:16:LEU:HG	2:D:31:LEU:HD11	1.78	0.63
1:A:39:ARG:NH2	1:A:112:GLU:C	2.52	0.63
2:D:35:ILE:HG22	2:D:54:PHE:HB3	1.80	0.63
2:D:363:LYS:O	2:D:364:LEU:HB2	1.98	0.63
2:D:237:LEU:HD22	2:D:237:LEU:N	2.13	0.63
1:A:17:ASP:CB	1:A:28:ARG:HD2	2.29	0.63
1:A:416:HIS:CE1	1:A:418:THR:HG23	2.32	0.63
1:A:384:LYS:HB2	1:A:409:GLN:CG	2.28	0.63
2:D:191:ASP:HB3	2:D:320:PRO:HD2	1.81	0.63
2:D:8:GLY:H	2:D:77:ALA:HB2	1.64	0.62
2:D:9:TYR:H	2:D:77:ALA:HB2	1.63	0.62
2:D:201:ASP:HA	2:D:204:ILE:HG22	1.81	0.62
1:A:207:MET:CE	1:A:211:VAL:HG21	2.29	0.62
2:D:169:TYR:O	2:D:173:VAL:HG23	2.00	0.62
1:A:200:ILE:HG12	1:A:201:GLY:N	2.11	0.62
1:A:239:GLU:O	1:A:243:THR:HG23	2.00	0.62
1:A:36:PRO:HD2	1:A:47:ILE:HD12	1.82	0.61
2:D:94:SER:O	2:D:95:VAL:HB	2.00	0.61
1:A:392:THR:OG1	1:A:402:GLU:CB	2.47	0.61
2:D:123:PRO:HA	2:D:161:PRO:HA	1.83	0.61
2:D:198:MET:SD	2:D:203:MET:HB2	2.41	0.60
1:A:232:ASN:HB3	1:A:233:PRO:CD	2.27	0.60
2:D:95:VAL:O	2:D:96:SER:CB	2.49	0.60
1:A:329:MET:O	1:A:333:THR:HG23	2.01	0.60
2:D:125:PHE:CE1	2:D:134:GLU:HG3	2.37	0.60
2:D:292:TYR:CZ	2:D:371:LYS:HE2	2.35	0.60
2:D:23:TRP:HZ3	2:D:145:LEU:HD12	1.65	0.60
1:A:90:TRP:HH2	2:D:171:SER:HB2	1.65	0.59
2:D:86:ARG:HD3	2:D:88:TYR:CE1	2.37	0.59
2:D:52:LEU:HB3	2:D:107:ILE:CG2	2.33	0.59
2:D:96:SER:O	2:D:97:VAL:HG23	2.03	0.59
2:D:118:LEU:HD22	2:D:119:LYS:N	2.17	0.59
2:D:246:ASP:H	2:D:247:PRO:CD	2.15	0.59
1:A:39:ARG:NH2	1:A:113:GLY:HA2	2.18	0.58
2:D:160:ILE:HD13	2:D:160:ILE:O	2.03	0.58
2:D:211:MET:O	2:D:326:PHE:HA	2.03	0.58
1:A:190:VAL:HG21	1:A:214:MET:HE1	1.84	0.58
2:D:343:ILE:HB	2:D:354:HIS:HB2	1.85	0.58
1:A:214:MET:CE	1:A:234:GLY:H	2.17	0.58
2:D:39:THR:HG22	2:D:51:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD22	1:A:455:LYS:CG	2.29	0.58
2:D:248:MET:HA	2:D:248:MET:CE	2.34	0.58
2:D:346:LEU:HA	2:D:351:SER:HA	1.86	0.58
1:A:345:THR:HG23	1:A:345:THR:O	2.04	0.57
1:A:326:ARG:HB3	1:A:339:TYR:CE2	2.40	0.57
1:A:157:ASN:HD22	1:A:158:PRO:HD2	1.67	0.57
1:A:199:THR:HG22	1:A:200:ILE:H	1.68	0.57
2:D:126:PRO:HG3	2:D:159:ASP:HB2	1.85	0.57
2:D:52:LEU:O	2:D:107:ILE:HG22	2.05	0.56
1:A:92:THR:HB	2:D:282:ALA:HB2	1.87	0.56
1:A:213:ASP:O	1:A:217:ILE:HG13	2.05	0.56
1:A:295:MET:O	1:A:299:MET:HG3	2.05	0.56
1:A:574:ILE:C	1:A:576:SER:H	2.08	0.56
2:D:279:ARG:HG3	2:D:289:ARG:O	2.06	0.56
2:D:362:THR:O	2:D:363:LYS:HB2	2.06	0.56
1:A:213:ASP:OD1	1:A:215:ALA:HB3	2.06	0.56
2:D:114:SER:O	2:D:115:ILE:HB	2.05	0.56
2:D:248:MET:HA	2:D:248:MET:HE2	1.88	0.56
2:D:117:ASN:HD21	2:D:165:THR:HG21	1.70	0.56
1:A:237:THR:CB	1:A:240:GLU:HG3	2.33	0.56
1:A:161:ARG:NH1	1:A:167:PRO:HD2	2.21	0.56
1:A:335:ASN:C	1:A:335:ASN:ND2	2.59	0.56
2:D:5:GLN:H	2:D:78:ASN:HD21	1.54	0.55
2:D:23:TRP:C	2:D:25:ASN:H	2.09	0.55
2:D:134:GLU:O	2:D:138:VAL:HG23	2.05	0.55
2:D:31:LEU:O	2:D:33:ALA:N	2.39	0.55
1:A:28:ARG:NH1	1:A:52:LEU:O	2.39	0.55
2:D:54:PHE:CE2	2:D:105:ILE:HD12	2.41	0.55
2:D:338:TYR:O	2:D:357:MET:HB3	2.05	0.55
1:A:296:LEU:HD22	1:A:296:LEU:H	1.72	0.55
2:D:283:TYR:C	2:D:285:GLU:H	2.09	0.55
2:D:12:LEU:HD11	2:D:14:VAL:HG23	1.89	0.54
2:D:204:ILE:HG23	2:D:205:ASN:N	2.21	0.54
1:A:81:ARG:HG3	1:A:81:ARG:NH1	2.22	0.54
2:D:363:LYS:O	2:D:364:LEU:CB	2.56	0.54
2:D:8:GLY:H	2:D:77:ALA:CB	2.20	0.54
2:D:237:LEU:HD21	2:D:309:LYS:HB2	1.90	0.54
2:D:292:TYR:O	2:D:294:GLU:N	2.39	0.54
1:A:278:GLU:O	1:A:281:ALA:HB3	2.07	0.54
1:A:336:LEU:O	1:A:341:VAL:HB	2.07	0.54
1:A:242:THR:O	1:A:246:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:O	1:A:284:MET:HG2	2.07	0.54
2:D:362:THR:O	2:D:363:LYS:CB	2.56	0.54
1:A:30:ARG:HD2	1:A:114:PHE:H	1.73	0.54
2:D:154:ASN:O	2:D:180:VAL:HG23	2.08	0.54
1:A:110:ARG:HB3	1:A:117:PRO:O	2.07	0.53
1:A:384:LYS:HD2	4:A:621:HOH:O	2.07	0.53
2:D:114:SER:O	2:D:116:GLU:N	2.35	0.53
2:D:114:SER:C	2:D:116:GLU:H	2.11	0.53
1:A:89:LYS:HG3	1:A:90:TRP:N	2.22	0.53
2:D:95:VAL:O	2:D:96:SER:HB2	2.06	0.53
1:A:384:LYS:CB	1:A:409:GLN:HG2	2.36	0.53
1:A:375:LEU:CD2	1:A:455:LYS:HG2	2.30	0.53
1:A:22:LEU:CD1	2:D:259:LEU:HD23	2.38	0.53
1:A:256:ILE:O	1:A:258:SER:N	2.42	0.53
2:D:99:SER:O	2:D:100:LYS:CB	2.55	0.53
1:A:159:ASP:HB2	1:A:373:ARG:NH2	2.24	0.53
1:A:252:MET:SD	1:A:281:ALA:HB3	2.49	0.53
1:A:330:ILE:C	1:A:332:LEU:H	2.12	0.53
2:D:132:ILE:HD12	2:D:197:MET:CE	2.37	0.53
2:D:241:ASN:ND2	2:D:244:LYS:H	2.06	0.53
1:A:81:ARG:HB3	1:A:100:TYR:CZ	2.44	0.52
2:D:174:ARG:HH11	2:D:188:VAL:HB	1.74	0.52
2:D:201:ASP:HA	2:D:204:ILE:CG2	2.39	0.52
1:A:157:ASN:HD22	1:A:158:PRO:CD	2.22	0.52
1:A:159:ASP:O	1:A:483:ARG:NH1	2.42	0.52
1:A:176:MET:HG3	1:A:278:GLU:OE2	2.10	0.52
2:D:74:VAL:HB	2:D:316:PHE:CE1	2.45	0.52
2:D:283:TYR:O	2:D:286:MET:HG2	2.09	0.52
1:A:50:GLU:OE1	1:A:51:LYS:HG2	2.10	0.52
1:A:304:TRP:H	1:A:304:TRP:HD1	1.56	0.52
1:A:61:ILE:C	1:A:61:ILE:HD12	2.31	0.51
2:D:241:ASN:HD21	2:D:244:LYS:H	1.57	0.51
1:A:161:ARG:HH11	1:A:166:ILE:HG23	1.76	0.51
1:A:574:ILE:HG22	1:A:574:ILE:O	2.10	0.51
2:D:281:GLY:O	2:D:282:ALA:C	2.48	0.51
2:D:363:LYS:HG2	2:D:364:LEU:N	2.24	0.51
1:A:44:VAL:O	2:D:122:ARG:HG2	2.10	0.51
2:D:283:TYR:C	2:D:285:GLU:N	2.64	0.51
2:D:306:GLY:O	2:D:359:THR:N	2.44	0.51
1:A:304:TRP:CD1	1:A:304:TRP:N	2.77	0.51
2:D:86:ARG:HG2	2:D:86:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:PHE:CE1	2:D:297:ARG:HA	2.46	0.51
1:A:103:ILE:HD13	1:A:127:ASN:HA	1.93	0.51
1:A:124:ARG:CG	1:A:124:ARG:HH21	2.24	0.51
2:D:203:MET:HA	2:D:206:GLN:HE21	1.75	0.51
1:A:199:THR:CG2	1:A:200:ILE:N	2.74	0.51
1:A:339:TYR:N	1:A:339:TYR:CD2	2.79	0.51
1:A:207:MET:HE2	1:A:211:VAL:HG21	1.93	0.50
1:A:425:SER:OG	1:A:427:SER:HB3	2.10	0.50
2:D:78:ASN:N	2:D:78:ASN:HD22	2.07	0.50
2:D:86:ARG:NH2	4:D:508:HOH:O	2.44	0.50
1:A:323:ARG:O	1:A:327:VAL:HG13	2.11	0.50
1:A:59:GLN:HB3	1:A:60:PRO:HD2	1.93	0.50
1:A:237:THR:CG2	1:A:238:MET:H	2.18	0.50
2:D:283:TYR:O	2:D:285:GLU:N	2.44	0.50
2:D:345:GLU:O	2:D:345:GLU:HG3	2.11	0.50
1:A:176:MET:HE1	1:A:278:GLU:CB	2.40	0.50
2:D:122:ARG:HG3	2:D:124:PHE:CE2	2.47	0.50
2:D:212:ILE:O	2:D:230:LEU:HA	2.12	0.50
1:A:214:MET:HG3	1:A:232:ASN:OD1	2.11	0.50
2:D:10:PRO:C	2:D:12:LEU:H	2.15	0.50
2:D:324:ILE:HD12	2:D:357:MET:HE2	1.94	0.50
2:D:174:ARG:NH1	2:D:188:VAL:O	2.45	0.50
1:A:300:LEU:C	1:A:302:GLY:H	2.15	0.49
2:D:199:ASP:N	2:D:202:MET:HE3	2.16	0.49
1:A:316:TRP:HH2	1:A:327:VAL:HG21	1.74	0.49
2:D:76:ASN:N	2:D:76:ASN:HD22	2.09	0.49
2:D:162:TRP:CZ2	2:D:169:TYR:HA	2.47	0.49
1:A:131:VAL:HG23	1:A:132:LEU:N	2.27	0.49
1:A:193:ASP:O	1:A:195:GLU:N	2.41	0.49
1:A:261:LYS:HD3	1:A:290:ALA:HB1	1.95	0.49
2:D:216:PRO:HD3	2:D:232:TYR:HB3	1.95	0.49
1:A:289:VAL:C	1:A:291:LYS:H	2.15	0.49
1:A:339:TYR:N	1:A:339:TYR:HD2	2.10	0.49
1:A:200:ILE:HD11	1:A:236:ILE:HG12	1.94	0.49
1:A:11:PHE:CD1	1:A:11:PHE:C	2.86	0.49
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.78	0.49
2:D:35:ILE:HG13	2:D:35:ILE:O	2.11	0.49
2:D:56:ASP:OD2	2:D:60:ILE:N	2.44	0.49
1:A:230:THR:O	1:A:231:GLY:O	2.30	0.49
1:A:296:LEU:HD22	1:A:296:LEU:N	2.27	0.49
1:A:231:GLY:O	1:A:232:ASN:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ASN:N	2:D:78:ASN:ND2	2.61	0.48
2:D:258:PHE:H	2:D:280:SER:HB3	1.77	0.48
2:D:374:ASN:HD22	2:D:375:GLU:N	2.11	0.48
1:A:330:ILE:HD13	1:A:336:LEU:CD1	2.44	0.48
2:D:23:TRP:O	2:D:25:ASN:N	2.41	0.48
2:D:95:VAL:HG22	2:D:96:SER:N	2.27	0.48
1:A:22:LEU:HD12	1:A:26:ARG:CZ	2.43	0.48
1:A:262:VAL:C	1:A:264:PRO:HD2	2.34	0.48
1:A:263:GLY:N	1:A:264:PRO:CD	2.76	0.48
1:A:571:ARG:HH21	1:A:577:VAL:HG22	1.78	0.48
2:D:199:ASP:OD2	2:D:199:ASP:C	2.51	0.48
1:A:569:GLY:O	1:A:570:SER:C	2.52	0.48
2:D:41:ARG:NE	2:D:341:GLU:OE2	2.47	0.48
2:D:363:LYS:CG	2:D:364:LEU:N	2.77	0.48
1:A:121:TYR:HA	1:A:122:PRO:C	2.34	0.48
1:A:127:ASN:OD1	1:A:129:THR:N	2.46	0.48
2:D:246:ASP:H	2:D:247:PRO:HD2	1.79	0.48
2:D:319:THR:O	2:D:322:VAL:HG22	2.13	0.48
2:D:98:ASP:CB	2:D:102:ASP:H	2.27	0.47
1:A:152:LEU:HD22	1:A:378:GLU:HG2	1.95	0.47
1:A:159:ASP:HB2	1:A:373:ARG:HH22	1.79	0.47
1:A:327:VAL:O	1:A:330:ILE:N	2.47	0.47
1:A:330:ILE:C	1:A:332:LEU:N	2.67	0.47
1:A:117:PRO:HG2	1:A:118:THR:H	1.79	0.47
2:D:5:GLN:HE21	2:D:5:GLN:HA	1.80	0.47
1:A:195:GLU:HB3	1:A:197:TYR:CD2	2.50	0.47
1:A:280:MET:HB3	1:A:284:MET:HE3	1.96	0.47
1:A:534:LEU:HD12	1:A:535:SER:N	2.30	0.47
2:D:93:PHE:HA	2:D:106:ALA:O	2.14	0.47
2:D:97:VAL:CG1	2:D:98:ASP:N	2.60	0.47
2:D:300:THR:HA	2:D:303:GLN:HE21	1.80	0.47
1:A:50:GLU:OE1	1:A:50:GLU:N	2.48	0.47
1:A:66:MET:O	1:A:67:SER:C	2.53	0.47
1:A:200:ILE:CG1	1:A:201:GLY:H	2.19	0.47
1:A:327:VAL:HG23	1:A:328:THR:N	2.30	0.47
1:A:468:ASP:CG	1:A:469:ASN:H	2.17	0.47
2:D:44:LEU:HD12	2:D:189:TRP:CD2	2.50	0.47
2:D:156:TYR:O	2:D:157:VAL:HG23	2.15	0.47
1:A:156:ILE:N	1:A:457:ASN:HD21	2.00	0.47
2:D:254:TYR:HB2	2:D:276:VAL:HG22	1.97	0.47
1:A:561:SER:HB2	1:A:565:TYR:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:PHE:HB3	2:D:107:ILE:HG13	1.97	0.47
1:A:308:TYR:CD1	1:A:332:LEU:HB2	2.50	0.46
2:D:201:ASP:C	2:D:204:ILE:HG22	2.36	0.46
1:A:320:THR:O	1:A:321:LYS:O	2.33	0.46
1:A:522:VAL:HG22	1:A:522:VAL:O	2.15	0.46
1:A:198:PRO:HB2	1:A:206:ILE:HB	1.97	0.46
1:A:561:SER:HB2	1:A:565:TYR:CD1	2.50	0.46
2:D:216:PRO:O	2:D:217:SER:HB3	2.14	0.46
1:A:571:ARG:HG2	1:A:572:ILE:N	2.30	0.46
1:A:81:ARG:HH22	1:A:102:GLY:N	2.13	0.46
2:D:167:GLU:CD	2:D:167:GLU:H	2.17	0.46
1:A:130:ASN:ND2	1:A:394:GLU:OE1	2.47	0.46
2:D:129:GLY:O	2:D:133:LYS:HG3	2.16	0.46
2:D:170:LEU:HD22	2:D:188:VAL:HG11	1.97	0.46
2:D:5:GLN:HA	2:D:5:GLN:NE2	2.30	0.46
2:D:51:MET:CE	2:D:53:GLN:HB3	2.46	0.46
2:D:253:ILE:HG12	2:D:275:ILE:HB	1.97	0.46
1:A:308:TYR:N	1:A:331:ILE:HD11	2.30	0.46
2:D:17:PHE:HB3	2:D:22:ALA:HB3	1.98	0.46
2:D:90:CYS:CB	2:D:107:ILE:HD11	2.34	0.46
2:D:288:TYR:CZ	2:D:371:LYS:HD3	2.51	0.46
1:A:39:ARG:HH21	1:A:39:ARG:HG3	1.80	0.46
1:A:48:PRO:CD	1:A:51:LYS:HG3	2.41	0.46
2:D:114:SER:C	2:D:116:GLU:N	2.68	0.46
1:A:43:ASP:O	2:D:122:ARG:HD3	2.16	0.45
1:A:133:ASN:HD21	1:A:392:THR:N	2.08	0.45
1:A:425:SER:C	1:A:427:SER:N	2.69	0.45
1:A:133:ASN:ND2	1:A:392:THR:HB	2.30	0.45
2:D:281:GLY:O	2:D:284:SER:N	2.43	0.45
2:D:333:PHE:CD1	2:D:333:PHE:N	2.85	0.45
1:A:324:ALA:O	1:A:327:VAL:HG22	2.17	0.45
2:D:51:MET:HE2	2:D:53:GLN:HB3	1.99	0.45
1:A:152:LEU:HD11	1:A:380:VAL:HG12	1.99	0.45
2:D:17:PHE:N	2:D:17:PHE:CD1	2.85	0.45
2:D:20:TYR:CE2	2:D:143:ARG:HA	2.52	0.45
2:D:144:THR:O	2:D:147:THR:HG23	2.17	0.45
1:A:39:ARG:NH2	1:A:112:GLU:O	2.39	0.45
1:A:9:ASN:O	1:A:85:HIS:HA	2.17	0.45
2:D:78:ASN:HD22	2:D:78:ASN:H	1.63	0.45
1:A:425:SER:C	1:A:427:SER:H	2.21	0.44
2:D:12:LEU:HD11	2:D:14:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:ASP:CA	2:D:204:ILE:HG22	2.44	0.44
2:D:369:PRO:O	2:D:370:VAL:O	2.35	0.44
1:A:327:VAL:HG12	1:A:339:TYR:OH	2.18	0.44
1:A:420:THR:HG23	1:A:433:LYS:O	2.18	0.44
2:D:23:TRP:C	2:D:25:ASN:N	2.71	0.44
2:D:46:GLY:HA3	2:D:174:ARG:NH2	2.32	0.44
2:D:76:ASN:N	2:D:76:ASN:ND2	2.64	0.44
1:A:34:LEU:HD13	1:A:35:HIS:CD2	2.53	0.44
1:A:92:THR:HB	2:D:282:ALA:CB	2.48	0.44
1:A:214:MET:HG3	1:A:232:ASN:O	2.17	0.44
1:A:441:ILE:HD12	1:A:441:ILE:N	2.32	0.44
2:D:246:ASP:N	2:D:247:PRO:CD	2.79	0.44
2:D:279:ARG:HA	2:D:279:ARG:HD3	1.72	0.44
1:A:202:ILE:O	1:A:202:ILE:HG22	2.18	0.44
1:A:237:THR:CG2	1:A:238:MET:N	2.73	0.44
1:A:257:LYS:O	1:A:258:SER:CB	2.66	0.44
1:A:343:VAL:HG13	1:A:343:VAL:O	2.18	0.44
1:A:19:MET:HE1	4:A:660:HOH:O	2.17	0.44
1:A:90:TRP:HZ3	2:D:168:ASN:ND2	2.16	0.44
1:A:404:ASP:O	1:A:410:GLU:HA	2.18	0.44
2:D:189:TRP:HH2	2:D:198:MET:HB3	1.83	0.44
2:D:290:ASN:OD1	2:D:372:VAL:HB	2.18	0.44
1:A:190:VAL:HA	1:A:199:THR:O	2.18	0.44
1:A:534:LEU:HD21	1:A:536:TRP:HE1	1.81	0.44
2:D:17:PHE:CE2	2:D:28:PHE:HB3	2.53	0.44
2:D:324:ILE:HD12	2:D:357:MET:CE	2.47	0.44
1:A:184:GLU:OE2	1:A:323:ARG:NH1	2.51	0.44
1:A:323:ARG:CA	1:A:326:ARG:HH21	2.24	0.44
2:D:87:ILE:HD13	2:D:146:LEU:HD22	1.99	0.44
1:A:243:THR:OG1	1:A:244:LEU:N	2.50	0.43
1:A:429:ARG:HG2	1:A:430:ARG:N	2.32	0.43
2:D:204:ILE:CG2	2:D:205:ASN:N	2.81	0.43
1:A:225:VAL:HG12	1:A:225:VAL:O	2.18	0.43
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.79	0.43
1:A:498:VAL:HG11	1:A:502:VAL:CG2	2.49	0.43
1:A:31:VAL:CB	1:A:34:LEU:HD11	2.39	0.43
1:A:38:GLN:CD	1:A:38:GLN:N	2.67	0.43
1:A:46:GLY:C	1:A:47:ILE:HG13	2.39	0.43
1:A:246:GLU:O	1:A:249:LEU:HB3	2.18	0.43
2:D:103:ASN:O	2:D:104:ILE:C	2.57	0.43
2:D:113:HIS:ND1	2:D:113:HIS:N	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:THR:HA	2:D:267:THR:HA	1.99	0.43
2:D:41:ARG:HG3	2:D:343:ILE:HG12	2.00	0.43
2:D:189:TRP:CE2	2:D:196:ASN:HB2	2.54	0.43
2:D:330:LYS:O	2:D:331:ASN:C	2.57	0.43
1:A:18:ARG:NH1	1:A:77:VAL:HG12	2.24	0.43
1:A:326:ARG:HE	1:A:326:ARG:HB2	1.60	0.43
1:A:174:MET:HE2	1:A:179:MET:HB2	2.01	0.43
1:A:327:VAL:CG2	1:A:328:THR:N	2.82	0.43
1:A:424:VAL:HA	1:A:429:ARG:O	2.18	0.43
2:D:205:ASN:HD22	2:D:205:ASN:C	2.22	0.43
2:D:374:ASN:HD22	2:D:374:ASN:C	2.22	0.43
1:A:38:GLN:N	1:A:38:GLN:HE21	2.13	0.43
2:D:279:ARG:HH11	2:D:279:ARG:HG2	1.83	0.43
1:A:157:ASN:HD22	1:A:157:ASN:C	2.22	0.43
1:A:492:GLY:C	1:A:493:ASN:HD22	2.21	0.43
2:D:107:ILE:HG23	2:D:109:LEU:CD1	2.48	0.43
2:D:155:ALA:HA	2:D:179:ALA:HA	2.01	0.43
2:D:160:ILE:HG12	2:D:161:PRO:O	2.19	0.43
1:A:227:ARG:HH21	1:A:229:ILE:HG12	1.84	0.42
1:A:439:TYR:HB3	1:A:441:ILE:CD1	2.49	0.42
1:A:550:TRP:CD1	1:A:550:TRP:C	2.92	0.42
1:A:571:ARG:HE	1:A:577:VAL:HG13	1.84	0.42
2:D:10:PRO:C	2:D:12:LEU:N	2.73	0.42
2:D:306:GLY:O	2:D:358:PHE:HA	2.19	0.42
1:A:312:ARG:C	1:A:314:SER:H	2.23	0.42
1:A:313:ASP:OD1	1:A:313:ASP:O	2.37	0.42
2:D:117:ASN:HD22	2:D:165:THR:HG21	1.81	0.42
1:A:193:ASP:C	1:A:195:GLU:H	2.22	0.42
2:D:107:ILE:HG23	2:D:109:LEU:HD11	2.01	0.42
2:D:160:ILE:HD13	2:D:160:ILE:H	1.84	0.42
2:D:251:ALA:HB2	2:D:273:ASN:HB2	2.01	0.42
2:D:313:ILE:O	2:D:314:GLY:C	2.58	0.42
1:A:316:TRP:CH2	1:A:327:VAL:HG21	2.53	0.42
1:A:116:ASP:OD2	1:A:116:ASP:C	2.58	0.42
2:D:210:PRO:HA	2:D:325:ILE:O	2.19	0.42
2:D:228:TYR:HB3	2:D:229:PRO:HD2	2.00	0.42
1:A:373:ARG:HG3	1:A:373:ARG:O	2.19	0.42
1:A:395:THR:OG1	1:A:399:HIS:HB2	2.20	0.42
1:A:30:ARG:HD2	1:A:114:PHE:N	2.34	0.42
1:A:39:ARG:NH2	1:A:113:GLY:CA	2.82	0.42
2:D:21:ASP:O	2:D:25:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:O	1:A:319:GLN:HG2	2.19	0.42
1:A:330:ILE:HD13	1:A:336:LEU:HD12	2.01	0.42
1:A:317:TYR:O	1:A:318:GLN:C	2.58	0.42
2:D:101:GLY:O	2:D:102:ASP:CB	2.68	0.42
1:A:506:VAL:O	1:A:506:VAL:CG2	2.67	0.41
1:A:257:LYS:O	1:A:258:SER:HB2	2.20	0.41
1:A:296:LEU:H	1:A:296:LEU:CD2	2.33	0.41
1:A:335:ASN:OD1	1:A:337:GLU:HG3	2.19	0.41
1:A:383:TYR:CD1	1:A:383:TYR:C	2.93	0.41
1:A:482:VAL:O	1:A:482:VAL:HG23	2.20	0.41
2:D:96:SER:O	2:D:97:VAL:CB	2.68	0.41
2:D:201:ASP:O	2:D:205:ASN:ND2	2.54	0.41
2:D:292:TYR:CE1	2:D:371:LYS:HG2	2.56	0.41
2:D:347:SER:C	2:D:349:ASN:H	2.23	0.41
1:A:278:GLU:O	1:A:281:ALA:N	2.52	0.41
1:A:409:GLN:O	1:A:410:GLU:C	2.57	0.41
2:D:153:ILE:HG21	2:D:202:MET:HE1	2.01	0.41
1:A:200:ILE:CD1	1:A:236:ILE:HG12	2.51	0.41
1:A:326:ARG:NH1	4:A:609:HOH:O	2.54	0.41
1:A:176:MET:HE3	1:A:180:LEU:HD21	2.03	0.41
2:D:71:GLN:HE21	2:D:71:GLN:HB2	1.65	0.41
2:D:195:VAL:O	2:D:195:VAL:HG12	2.21	0.41
1:A:107:LYS:HD2	1:A:125:LEU:HD23	2.03	0.41
1:A:245:PHE:O	1:A:246:GLU:C	2.57	0.41
1:A:407:PRO:C	1:A:409:GLN:H	2.22	0.41
2:D:96:SER:O	2:D:97:VAL:CG2	2.68	0.41
1:A:292:PHE:O	1:A:293:ASN:C	2.59	0.41
1:A:133:ASN:HD22	1:A:133:ASN:HA	1.65	0.41
1:A:186:LEU:HD21	1:A:238:MET:SD	2.61	0.41
2:D:44:LEU:O	2:D:44:LEU:HG	2.21	0.41
1:A:124:ARG:CG	1:A:124:ARG:NH2	2.81	0.41
1:A:571:ARG:C	1:A:572:ILE:HG13	2.40	0.41
2:D:52:LEU:HB3	2:D:107:ILE:HG22	2.03	0.41
2:D:122:ARG:O	2:D:124:PHE:CE2	2.74	0.41
2:D:174:ARG:NH1	2:D:188:VAL:HB	2.35	0.41
2:D:315:ASN:HD21	2:D:317:ASN:HB2	1.84	0.41
1:A:262:VAL:C	1:A:264:PRO:CD	2.88	0.40
2:D:347:SER:O	2:D:349:ASN:N	2.54	0.40
2:D:5:GLN:O	2:D:6:ARG:C	2.59	0.40
1:A:89:LYS:HD2	1:A:90:TRP:CE2	2.56	0.40
2:D:76:ASN:ND2	2:D:79:ASP:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ILE:O	2:D:114:SER:O	2.40	0.40
2:D:143:ARG:O	2:D:145:LEU:N	2.54	0.40
1:A:199:THR:CG2	1:A:200:ILE:H	2.33	0.40
2:D:47:ARG:O	2:D:48:ASN:ND2	2.55	0.40
2:D:114:SER:OG	2:D:167:GLU:HG2	2.22	0.40
1:A:183:ASP:HB3	1:A:323:ARG:HE	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/584 (98%)	474 (83%)	78 (14%)	19 (3%)	4	20
2	D	364/391 (93%)	288 (79%)	45 (12%)	31 (8%)	1	4
All	All	935/975 (96%)	762 (82%)	123 (13%)	50 (5%)	2	12

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	A	293	ASN
1	A	321	LYS
1	A	355	ALA
2	D	32	ALA
2	D	58	LYS
2	D	95	VAL
2	D	96	SER
2	D	97	VAL
2	D	100	LYS
2	D	103	ASN
2	D	104	ILE

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Mol	Chain	Res	Type
2	D	363	LYS
2	D	364	LEU
2	D	367	ILE
2	D	370	VAL
1	A	165	GLU
1	A	200	ILE
1	A	231	GLY
1	A	301	ALA
1	A	522	VAL
2	D	33	ALA
2	D	79	ASP
2	D	102	ASP
2	D	144	THR
2	D	243	HIS
2	D	292	TYR
2	D	293	GLU
2	D	362	THR
1	A	113	GLY
1	A	290	ALA
1	A	345	THR
2	D	77	ALA
2	D	99	SER
2	D	225	GLU
2	D	245	ARG
1	A	257	LYS
1	A	353	MET
1	A	357	VAL
2	D	24	SER
2	D	25	ASN
2	D	98	ASP
1	A	194	THR
1	A	294	THR
2	D	246	ASP
2	D	284	SER
2	D	348	ASN
1	A	208	LYS
1	A	574	ILE
2	D	314	GLY

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	448/494 (91%)	402 (90%)	46 (10%)	7	26
2	D	282/350 (81%)	257 (91%)	25 (9%)	9	34
All	All	730/844 (86%)	659 (90%)	71 (10%)	8	30

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	9	ASN
1	A	12	VAL
1	A	34	LEU
1	A	38	GLN
1	A	50	GLU
1	A	62	THR
1	A	66	MET
1	A	86	PHE
1	A	93	ASN
1	A	124	ARG
1	A	129	THR
1	A	133	ASN
1	A	153	ASP
1	A	157	ASN
1	A	173	ASN
1	A	184	GLU
1	A	188	LEU
1	A	195	GLU
1	A	251	ASP
1	A	252	MET
1	A	331	ILE
1	A	335	ASN
1	A	339	TYR
1	A	373	ARG
1	A	375	LEU
1	A	397	SER

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Mol	Chain	Res	Type
1	A	409	GLN
1	A	427	SER
1	A	432	ARG
1	A	437	ASN
1	A	440	ASP
1	A	442	THR
1	A	466	ASN
1	A	470	ARG
1	A	479	THR
1	A	487	THR
1	A	498	VAL
1	A	506	VAL
1	A	519	THR
1	A	522	VAL
1	A	527	THR
1	A	546	VAL
1	A	551	THR
1	A	554	MET
1	A	578	ASP
2	D	16	LEU
2	D	21	ASP
2	D	30	GLU
2	D	76	ASN
2	D	90	CYS
2	D	113	HIS
2	D	117	ASN
2	D	134	GLU
2	D	147	THR
2	D	154	ASN
2	D	160	ILE
2	D	168	ASN
2	D	183	ASP
2	D	198	MET
2	D	205	ASN
2	D	236	TRP
2	D	248	MET
2	D	267	THR
2	D	289	ARG
2	D	310	CYS
2	D	313	ILE
2	D	315	ASN
2	D	357	MET

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Mol	Chain	Res	Type
2	D	368	ASP
2	D	374	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	38	GLN
1	A	59	GLN
1	A	93	ASN
1	A	120	GLN
1	A	133	ASN
1	A	151	ASN
1	A	157	ASN
1	A	173	ASN
1	A	293	ASN
1	A	335	ASN
1	A	443	ASN
1	A	457	ASN
1	A	469	ASN
1	A	473	GLN
1	A	493	ASN
2	D	5	GLN
2	D	25	ASN
2	D	71	GLN
2	D	76	ASN
2	D	78	ASN
2	D	117	ASN
2	D	154	ASN
2	D	168	ASN
2	D	205	ASN
2	D	241	ASN
2	D	273	ASN
2	D	303	GLN
2	D	315	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NEN	A	607	1	9,9,9	1.19	1 (11%)	12,12,12	4.58	9 (75%)

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
3	NEN	A	607	1	-	2/2/15/15	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	NEN	C3-N1	2.00	1.41	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	NEN	C3-N1-C2	-8.81	108.92	112.96
3	A	607	NEN	O1-C2-N1	8.26	133.07	123.92
3	A	607	NEN	C5-N1-C2	5.48	129.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	NEN	O2-C3-N1	4.80	129.23	123.92
3	A	607	NEN	O1-C2-C1	-4.34	116.00	127.08
3	A	607	NEN	C1-C2-N1	3.15	110.92	108.00
3	A	607	NEN	O2-C3-C4	-2.67	120.25	127.08
3	A	607	NEN	C4-C3-N1	2.61	110.42	108.00
3	A	607	NEN	C5-N1-C3	-2.07	119.89	122.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	607	NEN	C6-C5-N1-C2
3	A	607	NEN	C6-C5-N1-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	573/584 (98%)	-0.10	6 (1%) 82 69	9, 40, 85, 161	0
2	D	368/391 (94%)	0.15	16 (4%) 35 17	24, 65, 112, 128	0
All	All	941/975 (96%)	-0.01	22 (2%) 60 39	9, 49, 106, 161	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	4.9
2	D	99	SER	4.7
2	D	98	ASP	4.6
1	A	349	SER	4.3
1	A	351	LEU	4.2
1	A	350	LEU	3.1
1	A	348	ARG	2.9
2	D	326	PHE	2.8
2	D	311	SER	2.8
2	D	97	VAL	2.6
2	D	337	PHE	2.5
2	D	234	PHE	2.4
1	A	347	ALA	2.4
2	D	102	ASP	2.4
2	D	7	PRO	2.3
2	D	211	MET	2.3
2	D	347	SER	2.3
2	D	318	LEU	2.2
2	D	216	PRO	2.1
2	D	331	ASN	2.1
2	D	217	SER	2.0
2	D	100	LYS	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 monosaccharides 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(\AA^2)	Q<0.9
3	NEN	A	607	9/9	0.81	0.26	103,107,109,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.