



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:08 pm BST

PDB ID : 1N80
Title : Bacteriophage T4 baseplate structural protein gp8
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Deposited on : 2002-11-18
Resolution : 2.45 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

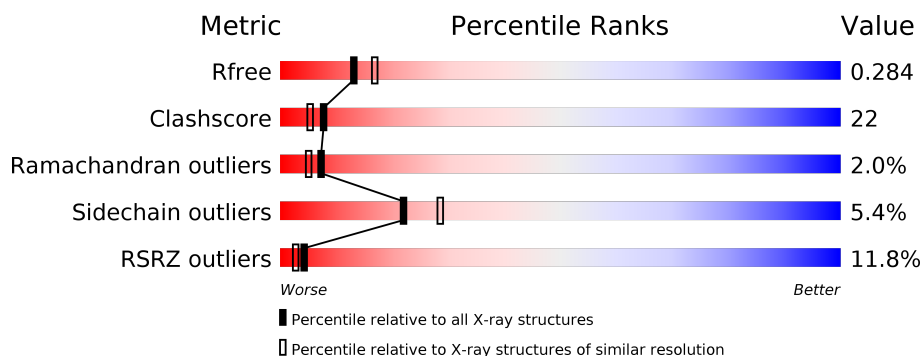
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	334	
1	B	334	
1	C	334	
1	D	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	337	-	-	X	-
2	CL	A	344	-	-	-	X
2	CL	B	336	-	-	X	-
2	CL	C	336	-	-	X	-
2	CL	C	337	-	-	X	-
2	CL	C	342	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11016 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 baseplate structural protein gp8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	B	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	C	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			
1	D	328	Total	C	N	O	S	0	0	0
			2631	1677	430	507	17			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cl	0	0
			6	6		
2	A	10	Total	Cl	0	0
			10	10		
2	D	8	Total	Cl	0	0
			8	8		
2	C	8	Total	Cl	0	0
			8	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	75	Total	O	0	0
			75	75		
3	C	138	Total	O	0	0
			138	138		
3	D	108	Total	O	0	0
			108	108		

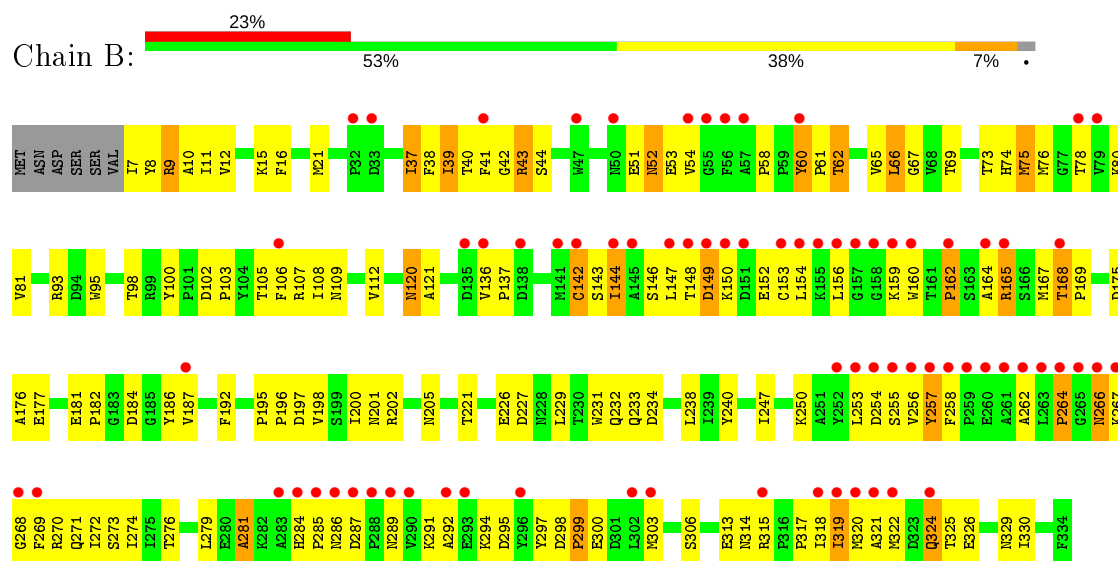
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: baseplate structural protein gp8

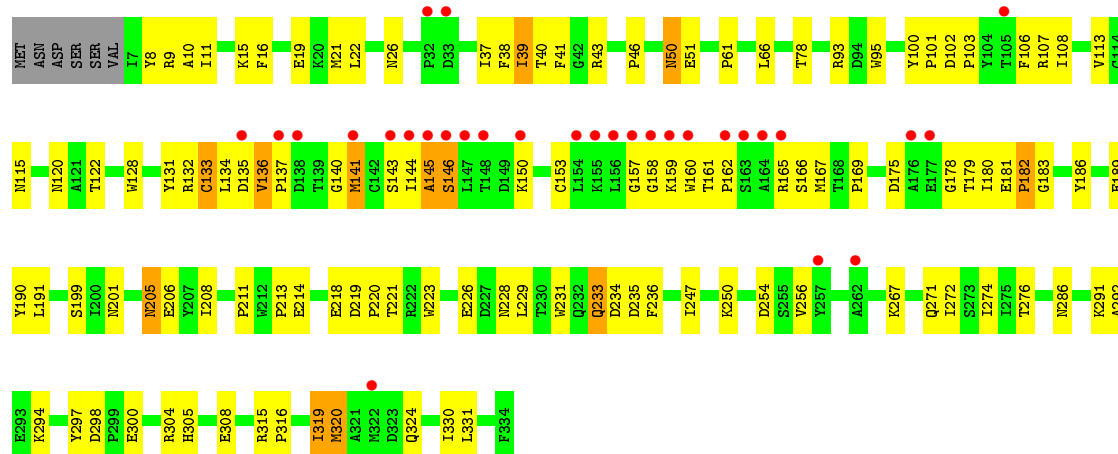


- Molecule 1: baseplate structural protein gp8

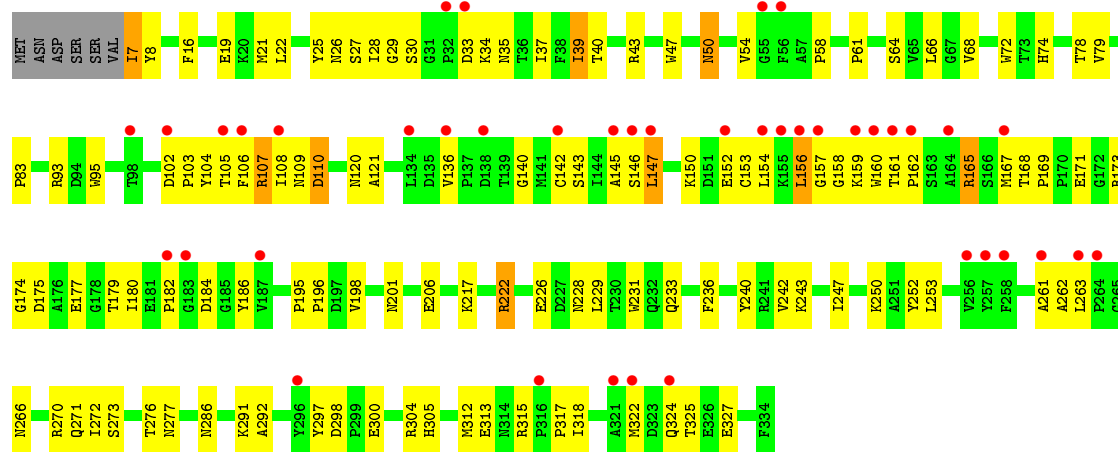


- Molecule 1: baseplate structural protein gp8





- Molecule 1: baseplate structural protein gp8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.87Å 66.78Å 82.16Å 93.11° 101.28° 90.77°	Depositor
Resolution (Å)	39.11 – 2.45 39.10 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.11-2.45) 97.3 (39.10-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.10 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.284 0.236 , 0.284	Depositor DCC
R_{free} test set	1286 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11016	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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:
CL

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	0.42	0/2709	0.66	1/3694 (0.0%)
1	B	0.38	0/2709	0.59	0/3694
1	C	0.41	0/2709	0.65	1/3694 (0.0%)
1	D	0.39	0/2709	0.62	0/3694
All	All	0.40	0/10836	0.63	2/14776 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	ASP	N-CA-C	-5.81	95.31	111.00
1	A	298	ASP	N-CA-C	-5.71	95.57	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2631	0	2509	85	0
1	B	2631	0	2509	148	0
1	C	2631	0	2509	122	0
1	D	2631	0	2509	122	0
2	A	10	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	4	0
2	C	8	0	0	5	0
2	D	8	0	0	1	0
3	A	139	0	0	2	0
3	B	75	0	0	2	0
3	C	138	0	0	7	0
3	D	108	0	0	4	0
All	All	11016	0	10036	449	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 22.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:SER:HB3	1:C:159:LYS:H	1.08	1.17
1:A:108:ILE:HD12	1:A:108:ILE:H	1.23	1.04
1:B:137:PRO:HG2	1:B:162:PRO:HB3	1.39	1.01
1:A:10:ALA:HB2	1:B:313:GLU:HG3	1.40	1.01
1:D:147:LEU:HD22	1:D:152:GLU:HB3	1.48	0.95
1:A:319:ILE:HD13	1:A:319:ILE:H	1.32	0.94
1:B:254:ASP:HA	1:B:325:THR:HG22	1.51	0.93
1:A:50:ASN:HD22	1:A:50:ASN:H	1.13	0.90
1:D:324:GLN:HG2	1:D:325:THR:H	1.34	0.90
1:B:221:THR:HG22	1:B:226:GLU:HB3	1.53	0.89
1:C:50:ASN:HD22	1:C:50:ASN:H	1.18	0.89
1:C:143:SER:HB3	1:C:159:LYS:N	1.90	0.86
1:C:107:ARG:HD2	1:C:159:LYS:HD2	1.57	0.86
1:B:107:ARG:HH11	1:B:159:LYS:HD2	1.41	0.85
1:B:37:ILE:HG23	1:B:81:VAL:HB	1.57	0.85
1:C:134:LEU:HG	1:C:189:GLU:HB2	1.58	0.85
1:B:37:ILE:HD11	1:B:274:ILE:HG23	1.58	0.84
1:D:93:ARG:HH22	1:D:106:PHE:HE1	1.21	0.84
1:A:319:ILE:CD1	1:A:319:ILE:H	1.93	0.82
1:D:175:ASP:HB3	1:D:179:THR:H	1.45	0.82
1:C:136:VAL:HB	1:C:137:PRO:HD2	1.61	0.81
1:A:201:ASN:O	1:A:250:LYS:HE3	1.79	0.81
1:C:205:ASN:ND2	1:C:206:GLU:HG3	1.97	0.79
1:A:108:ILE:CD1	1:A:108:ILE:H	1.97	0.78
1:B:39:ILE:HD13	1:B:40:THR:N	1.98	0.78
1:C:132:ARG:HB2	1:C:191:LEU:HD11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ALA:HB1	1:D:322:MET:HA	1.65	0.78
1:C:137:PRO:HG3	1:C:162:PRO:HB3	1.65	0.78
1:C:135:ASP:O	1:C:136:VAL:HG13	1.84	0.77
1:C:108:ILE:HD12	1:C:108:ILE:H	1.49	0.76
1:B:40:THR:HG22	1:B:78:THR:HG22	1.67	0.76
1:B:321:ALA:HB3	1:B:324:GLN:HB2	1.67	0.76
1:C:40:THR:HG22	1:C:78:THR:HG22	1.69	0.74
1:D:93:ARG:NH2	1:D:106:PHE:HE1	1.85	0.74
1:D:40:THR:HG22	1:D:78:THR:HG22	1.69	0.74
1:B:11:ILE:O	1:B:11:ILE:HD12	1.88	0.74
1:B:58:PRO:HG3	1:B:315:ARG:HA	1.70	0.74
1:B:40:THR:OG1	1:B:273:SER:HB3	1.88	0.73
1:B:284:HIS:HB2	1:B:287:ASP:OD2	1.88	0.73
1:B:102:ASP:HA	2:B:336:CL:CL	2.26	0.73
1:C:143:SER:CB	1:C:159:LYS:H	1.96	0.72
1:B:137:PRO:HG2	1:B:162:PRO:CB	2.18	0.72
1:D:58:PRO:HG3	1:D:315:ARG:HA	1.70	0.72
1:B:319:ILE:HD13	1:B:319:ILE:H	1.54	0.72
1:D:29:GLY:HA3	1:D:34:LYS:HD3	1.72	0.72
1:D:50:ASN:HD22	1:D:50:ASN:H	1.38	0.72
1:A:8:TYR:CE1	1:B:315:ARG:HD2	2.25	0.71
1:C:10:ALA:O	1:C:11:ILE:HG23	1.90	0.71
1:B:147:LEU:O	1:B:153:CYS:HB2	1.91	0.71
1:B:147:LEU:HD22	1:B:156:LEU:HD21	1.74	0.69
1:C:319:ILE:HD12	1:C:319:ILE:H	1.58	0.69
1:B:98:THR:HA	1:B:103:PRO:HG2	1.75	0.69
1:A:232:GLN:HE21	1:B:286:ASN:HA	1.56	0.69
1:A:108:ILE:HD12	1:A:108:ILE:N	2.03	0.69
1:A:120:ASN:O	1:A:122:THR:HG23	1.93	0.68
1:A:319:ILE:N	1:A:319:ILE:HD13	2.07	0.68
1:C:39:ILE:HD11	1:C:272:ILE:HG23	1.75	0.68
1:B:181:GLU:HG2	1:B:187:VAL:HG22	1.75	0.67
1:C:11:ILE:HD12	1:C:11:ILE:O	1.94	0.66
1:C:107:ARG:CD	1:C:159:LYS:HD2	2.25	0.66
1:B:75:MET:HB3	1:B:299:PRO:HB3	1.77	0.66
1:C:205:ASN:HD22	1:C:206:GLU:N	1.93	0.66
1:B:202:ARG:NH2	1:B:250:LYS:HG2	2.11	0.66
1:C:131:TYR:CD1	1:C:190:TYR:HA	2.31	0.66
1:D:182:PRO:HG2	1:D:184:ASP:OD1	1.95	0.66
1:D:263:LEU:HB2	1:D:266:ASN:HB3	1.77	0.66
1:C:131:TYR:HD1	1:C:190:TYR:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ILE:HG22	1:D:8:TYR:CD2	2.31	0.65
1:A:315:ARG:HB3	1:B:8:TYR:CD1	2.31	0.65
1:B:272:ILE:HB	1:B:313:GLU:HB3	1.79	0.64
1:B:329:ASN:O	1:B:330:ILE:HG13	1.97	0.64
1:D:324:GLN:HG2	1:D:325:THR:N	2.11	0.64
1:D:25:TYR:O	1:D:28:ILE:HD12	1.98	0.64
1:A:108:ILE:O	1:A:109:ASN:HB2	1.96	0.64
1:B:321:ALA:HB3	1:B:324:GLN:CB	2.26	0.64
1:C:141:MET:N	3:C:371:HOH:O	2.29	0.64
1:C:319:ILE:N	1:C:319:ILE:HD12	2.12	0.63
1:D:7:ILE:N	1:D:7:ILE:HD12	2.12	0.63
1:B:152:GLU:C	1:B:154:LEU:H	2.02	0.62
1:C:120:ASN:O	1:C:122:THR:HG23	1.99	0.62
1:A:10:ALA:HB2	1:B:313:GLU:CG	2.22	0.62
1:A:205:ASN:ND2	1:A:206:GLU:HG3	2.15	0.62
1:A:8:TYR:CD1	1:B:315:ARG:HD2	2.34	0.62
1:B:136:VAL:HB	1:B:162:PRO:HG2	1.81	0.62
1:B:7:ILE:HG23	1:B:8:TYR:N	2.14	0.62
1:D:222:ARG:HG2	1:D:222:ARG:HH21	1.65	0.62
1:B:95:TRP:HB3	1:B:120:ASN:HD21	1.65	0.61
1:C:221:THR:HA	1:C:226:GLU:OE1	2.00	0.61
1:B:182:PRO:HD2	1:B:186:TYR:O	2.00	0.61
1:D:39:ILE:HD13	1:D:40:THR:N	2.15	0.61
1:D:140:GLY:HA3	1:D:162:PRO:HA	1.83	0.61
1:D:50:ASN:N	1:D:50:ASN:HD22	1.95	0.61
1:D:102:ASP:OD2	1:D:105:THR:HB	2.01	0.61
1:B:147:LEU:HD22	1:B:156:LEU:CD2	2.31	0.61
1:A:10:ALA:O	1:A:11:ILE:HG23	2.00	0.61
1:B:146:SER:O	1:B:148:THR:HG23	2.01	0.61
1:C:145:ALA:O	1:C:146:SER:HB2	2.00	0.61
1:C:144:ILE:H	1:C:144:ILE:HD12	1.66	0.60
1:D:175:ASP:HB3	1:D:179:THR:N	2.14	0.60
1:A:50:ASN:HD22	1:A:50:ASN:N	1.92	0.60
1:D:150:LYS:HG3	1:D:160:TRP:CG	2.36	0.60
1:B:105:THR:HG22	1:B:165:ARG:HG2	1.84	0.59
1:B:254:ASP:CG	1:B:256:VAL:HG12	2.22	0.59
1:C:304:ARG:O	1:C:305:HIS:HB2	2.02	0.59
1:D:83:PRO:HG2	2:D:341:CL:CL	2.39	0.59
1:B:324:GLN:HE21	1:B:324:GLN:HA	1.67	0.59
1:A:22:LEU:HG	2:A:336:CL:CL	2.38	0.59
1:B:271:GLN:HG2	1:B:314:ASN:OD1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASP:CB	1:D:179:THR:HB	2.32	0.59
1:A:312:MET:HB2	1:B:11:ILE:HD11	1.83	0.59
1:D:50:ASN:ND2	1:D:50:ASN:H	2.00	0.59
1:A:321:ALA:HB3	1:A:324:GLN:HG3	1.84	0.59
1:A:315:ARG:HB3	1:B:8:TYR:HD1	1.67	0.59
1:D:107:ARG:HD2	1:D:107:ARG:N	2.17	0.59
1:A:132:ARG:HB2	1:A:191:LEU:HD11	1.84	0.59
1:B:231:TRP:HA	1:B:234:ASP:OD2	2.02	0.59
1:A:106:PHE:C	1:A:107:ARG:HD2	2.23	0.58
1:B:143:SER:O	1:B:144:ILE:HG23	2.03	0.58
1:C:134:LEU:CG	1:C:189:GLU:HB2	2.31	0.58
1:C:205:ASN:HD22	1:C:206:GLU:H	1.50	0.58
1:C:150:LYS:HA	1:C:160:TRP:CZ3	2.38	0.58
1:C:22:LEU:HG	2:C:336:CL:CL	2.41	0.58
1:D:175:ASP:HB2	1:D:179:THR:HB	1.84	0.58
1:B:221:THR:HG22	1:B:226:GLU:CB	2.31	0.57
1:B:7:ILE:HG23	1:B:8:TYR:H	1.69	0.57
1:C:205:ASN:HD21	1:C:206:GLU:HG3	1.68	0.57
1:A:107:ARG:HD2	1:A:107:ARG:N	2.18	0.57
1:C:267:LYS:N	1:C:267:LYS:HD2	2.19	0.57
1:D:201:ASN:O	1:D:250:LYS:HE3	2.02	0.57
1:A:114:CYS:HA	1:A:120:ASN:OD1	2.04	0.57
1:D:217:LYS:HG3	1:D:236:PHE:CE2	2.40	0.57
1:D:270:ARG:CZ	1:D:317:PRO:HB3	2.34	0.57
1:A:131:TYR:CD1	1:A:190:TYR:HA	2.40	0.57
1:A:40:THR:HG22	1:A:78:THR:HG22	1.86	0.57
1:A:9:ARG:HD2	1:B:60:TYR:CE2	2.40	0.57
1:D:252:TYR:HB3	1:D:325:THR:CG2	2.34	0.57
1:C:143:SER:OG	1:C:144:ILE:HD12	2.05	0.56
1:A:171:GLU:HA	3:A:360:HOH:O	2.05	0.56
1:D:107:ARG:HG2	1:D:159:LYS:HE3	1.86	0.56
1:B:98:THR:HA	1:B:103:PRO:CG	2.34	0.56
1:B:229:LEU:O	1:B:232:GLN:HG3	2.05	0.56
1:B:270:ARG:CZ	1:B:317:PRO:HB3	2.34	0.56
1:B:184:ASP:OD1	1:B:186:TYR:HB2	2.05	0.56
1:B:294:LYS:HB3	1:B:297:TYR:CE2	2.40	0.56
1:C:102:ASP:N	1:C:103:PRO:HD3	2.20	0.56
1:A:282:LYS:HD3	1:A:303:MET:CE	2.35	0.56
1:C:103:PRO:HD2	2:C:335:CL:CL	2.43	0.56
1:C:161:THR:O	3:C:371:HOH:O	2.17	0.56
1:B:192:PHE:CD2	1:B:238:LEU:HD21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASN:N	1:C:205:ASN:HD22	2.03	0.56
1:B:269:PHE:CE1	1:B:318:ILE:HB	2.40	0.56
1:B:108:ILE:O	1:B:109:ASN:HB2	2.05	0.56
1:B:149:ASP:C	1:B:150:LYS:HD2	2.25	0.56
1:A:50:ASN:H	1:A:50:ASN:ND2	1.93	0.55
1:B:279:LEU:HD13	1:B:289:ASN:HD22	1.69	0.55
1:A:197:ASP:OD1	1:A:222:ARG:NH1	2.39	0.55
1:A:7:ILE:HD12	1:A:7:ILE:N	2.22	0.55
1:C:10:ALA:HB2	1:D:313:GLU:HG3	1.87	0.55
1:C:39:ILE:HD13	1:C:40:THR:N	2.22	0.55
1:C:26:ASN:ND2	2:C:336:CL:CL	2.65	0.55
1:A:11:ILE:O	1:A:11:ILE:HD12	2.06	0.55
1:B:152:GLU:C	1:B:154:LEU:N	2.60	0.54
1:D:47:TRP:HE1	1:D:270:ARG:HB3	1.72	0.54
1:B:142:CYS:O	1:B:144:ILE:HG12	2.07	0.54
1:B:319:ILE:CD1	1:B:319:ILE:H	2.19	0.54
1:C:50:ASN:H	1:C:50:ASN:ND2	1.97	0.54
1:A:107:ARG:HH21	1:A:107:ARG:HG2	1.73	0.54
1:C:136:VAL:HB	1:C:137:PRO:CD	2.32	0.54
1:D:195:PRO:HG2	1:D:198:VAL:CG2	2.37	0.54
1:A:107:ARG:CB	1:A:159:LYS:HE2	2.38	0.54
1:B:142:CYS:SG	1:B:147:LEU:HB2	2.48	0.54
1:B:42:GLY:O	1:B:43:ARG:HB3	2.08	0.54
1:C:228:ASN:O	1:C:229:LEU:HD23	2.08	0.53
1:D:107:ARG:HH21	1:D:107:ARG:HG2	1.73	0.53
1:B:136:VAL:HB	1:B:137:PRO:HD2	1.90	0.53
1:B:153:CYS:SG	1:B:160:TRP:HE3	2.32	0.53
1:B:200:ILE:HG22	1:B:201:ASN:ND2	2.22	0.53
1:D:182:PRO:HD2	1:D:186:TYR:O	2.08	0.53
1:A:28:ILE:HG12	1:A:37:ILE:HD13	1.89	0.53
1:D:153:CYS:O	1:D:153:CYS:SG	2.67	0.53
1:A:19:GLU:OE1	1:B:276:THR:HG21	2.08	0.53
1:D:64:SER:O	1:D:68:VAL:HG23	2.08	0.53
1:B:10:ALA:O	1:B:11:ILE:HG23	2.08	0.53
1:C:101:PRO:C	1:C:103:PRO:HD3	2.29	0.53
1:A:117:ALA:HB1	1:A:118:PRO:HD2	1.91	0.53
1:A:95:TRP:CD2	1:A:169:PRO:HB3	2.42	0.53
1:A:76:MET:HE2	1:A:261:ALA:HB1	1.91	0.53
1:A:147:LEU:CD1	1:A:156:LEU:HD12	2.39	0.53
1:A:95:TRP:CH2	1:A:169:PRO:HD3	2.42	0.53
1:C:93:ARG:NH2	1:C:106:PHE:HE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:TYR:HB3	1:D:325:THR:HG21	1.91	0.53
1:A:233:GLN:HG3	1:A:234:ASP:N	2.24	0.53
1:D:95:TRP:HB3	1:D:120:ASN:OD1	2.09	0.53
1:B:21:MET:HG3	1:B:247:ILE:HG13	1.91	0.52
1:D:39:ILE:HD13	1:D:39:ILE:C	2.29	0.52
1:B:274:ILE:HD11	1:B:330:ILE:HD13	1.90	0.52
1:A:76:MET:CE	1:A:261:ALA:HB1	2.38	0.52
1:D:33:ASP:O	1:D:34:LYS:HG2	2.09	0.52
1:A:132:ARG:HH21	1:A:132:ARG:HG3	1.75	0.52
1:A:8:TYR:HE1	1:B:315:ARG:HD2	1.71	0.52
1:B:93:ARG:O	1:B:112:VAL:HG13	2.10	0.52
1:C:214:GLU:HB2	2:C:337:CL:CL	2.47	0.52
1:B:105:THR:HG23	2:B:336:CL:CL	2.47	0.52
1:A:232:GLN:NE2	1:B:286:ASN:HA	2.25	0.52
1:A:93:ARG:NH2	1:A:106:PHE:CE1	2.79	0.51
1:C:205:ASN:HB3	3:C:356:HOH:O	2.09	0.51
1:B:41:PHE:O	1:B:76:MET:HB2	2.11	0.51
1:C:132:ARG:HG3	1:C:132:ARG:HH21	1.75	0.51
1:C:137:PRO:HG3	1:C:162:PRO:CB	2.38	0.51
1:B:154:LEU:HD22	1:B:154:LEU:N	2.26	0.51
1:A:9:ARG:HB3	1:B:60:TYR:CD2	2.44	0.51
1:D:43:ARG:HA	1:D:74:HIS:HB3	1.92	0.51
1:A:282:LYS:NZ	1:A:289:ASN:OD1	2.44	0.51
1:C:100:TYR:HB3	1:C:101:PRO:HD2	1.92	0.51
1:D:40:THR:HG22	1:D:78:THR:CG2	2.37	0.51
1:A:234:ASP:OD1	1:A:241:ARG:HD2	2.10	0.51
1:D:147:LEU:HD13	1:D:152:GLU:O	2.11	0.51
1:C:61:PRO:HA	3:C:478:HOH:O	2.10	0.51
1:A:308:GLU:HG3	1:B:240:TYR:CE2	2.45	0.51
1:B:39:ILE:HD13	1:B:39:ILE:C	2.31	0.51
1:C:144:ILE:N	1:C:144:ILE:HD12	2.25	0.51
1:C:316:PRO:HD3	1:D:7:ILE:O	2.11	0.50
1:B:258:PHE:O	1:B:258:PHE:CD1	2.64	0.50
1:A:150:LYS:O	1:A:154:LEU:HD13	2.12	0.50
1:B:148:THR:O	1:B:149:ASP:HB2	2.11	0.50
1:B:41:PHE:HA	1:B:271:GLN:O	2.11	0.50
1:C:181:GLU:O	1:C:183:GLY:N	2.45	0.50
1:D:277:ASN:HA	1:D:291:LYS:HE3	1.93	0.50
1:C:136:VAL:CB	1:C:137:PRO:HD2	2.35	0.50
1:D:262:ALA:CB	1:D:322:MET:HA	2.39	0.50
1:B:254:ASP:OD2	1:B:256:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ASP:OD2	1:C:179:THR:HB	2.11	0.49
1:D:222:ARG:HG2	1:D:222:ARG:NH2	2.27	0.49
1:C:205:ASN:ND2	1:C:206:GLU:N	2.60	0.49
1:D:173:ARG:HH22	1:D:226:GLU:CD	2.15	0.49
1:B:11:ILE:HD12	1:B:11:ILE:C	2.31	0.49
1:A:9:ARG:HB3	1:B:60:TYR:HD2	1.75	0.49
1:C:201:ASN:O	1:C:250:LYS:CE	2.60	0.49
1:C:21:MET:HG3	1:C:247:ILE:HG13	1.95	0.49
1:D:107:ARG:HB3	1:D:159:LYS:HZ2	1.76	0.49
1:A:115:ASN:N	1:A:120:ASN:HB3	2.27	0.49
1:D:253:LEU:O	1:D:325:THR:HG23	2.12	0.49
1:D:324:GLN:CG	1:D:325:THR:H	2.16	0.49
1:D:206:GLU:OE2	1:D:206:GLU:N	2.45	0.49
1:D:108:ILE:O	1:D:109:ASN:HB2	2.13	0.49
1:B:303:MET:CG	1:B:306:SER:HB3	2.42	0.48
1:D:140:GLY:H	1:D:160:TRP:HZ2	1.61	0.48
1:A:321:ALA:HB3	1:A:324:GLN:CG	2.43	0.48
1:B:167:MET:HB2	3:B:341:HOH:O	2.13	0.48
1:B:303:MET:HA	2:B:340:CL:CL	2.50	0.48
1:B:294:LYS:HG3	1:B:295:ASP:N	2.27	0.48
1:A:205:ASN:HD21	1:A:206:GLU:HG3	1.78	0.48
1:B:37:ILE:HD11	1:B:274:ILE:CG2	2.37	0.48
1:D:304:ARG:O	1:D:305:HIS:HB2	2.14	0.48
1:C:16:PHE:O	1:C:19:GLU:HB3	2.12	0.48
1:A:173:ARG:HH22	1:A:226:GLU:CD	2.17	0.48
1:A:250:LYS:HG3	1:A:327:GLU:OE2	2.14	0.48
1:B:62:THR:O	1:B:67:GLY:HA3	2.14	0.48
1:B:262:ALA:HA	1:B:320:MET:HG3	1.95	0.48
1:C:108:ILE:HG13	1:C:136:VAL:HG21	1.94	0.48
1:C:181:GLU:C	1:C:183:GLY:H	2.17	0.48
1:D:250:LYS:NZ	1:D:327:GLU:OE1	2.47	0.48
1:C:235:ASP:O	1:C:236:PHE:HB2	2.14	0.48
1:D:174:GLY:HA3	1:D:180:ILE:CG1	2.44	0.47
1:C:143:SER:OG	1:C:158:GLY:HA3	2.13	0.47
1:B:37:ILE:HD13	1:B:38:PHE:N	2.29	0.47
1:C:107:ARG:HD2	1:C:159:LYS:CD	2.36	0.47
1:C:205:ASN:N	1:C:205:ASN:ND2	2.61	0.47
1:C:292:ALA:HB1	1:C:297:TYR:CE2	2.49	0.47
1:D:47:TRP:CD1	1:D:270:ARG:HD3	2.50	0.47
1:B:54:VAL:O	1:B:54:VAL:HG13	2.14	0.47
1:C:181:GLU:C	1:C:183:GLY:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:TYR:CE2	1:D:315:ARG:HB2	2.49	0.47
1:D:21:MET:HG3	1:D:247:ILE:HG13	1.96	0.47
1:A:65:VAL:HG23	2:A:337:CL:CL	2.52	0.47
1:B:73:THR:C	1:B:75:MET:H	2.18	0.47
1:B:154:LEU:C	1:B:156:LEU:H	2.18	0.47
1:A:232:GLN:HA	1:B:289:ASN:HD21	1.80	0.47
1:B:37:ILE:HD13	1:B:37:ILE:C	2.35	0.47
1:C:115:ASN:N	1:C:120:ASN:HB3	2.29	0.47
1:D:7:ILE:HG22	1:D:8:TYR:CE2	2.49	0.47
1:C:134:LEU:CD1	1:C:189:GLU:HB2	2.45	0.47
1:D:136:VAL:HG21	1:D:162:PRO:HD3	1.96	0.47
1:D:47:TRP:NE1	1:D:270:ARG:HB3	2.30	0.47
1:D:165:ARG:NH2	1:D:167:MET:HG2	2.30	0.47
1:D:150:LYS:HA	1:D:160:TRP:CE3	2.49	0.47
1:D:171:GLU:O	1:D:180:ILE:HD13	2.15	0.47
1:D:175:ASP:C	1:D:177:GLU:H	2.18	0.47
1:B:294:LYS:HG3	1:B:295:ASP:H	1.80	0.46
1:D:252:TYR:CE1	1:D:327:GLU:HB2	2.50	0.46
1:D:252:TYR:HE1	1:D:327:GLU:HB2	1.80	0.46
1:B:292:ALA:HB1	1:B:297:TYR:CE2	2.50	0.46
1:B:319:ILE:HD13	1:B:319:ILE:N	2.25	0.46
1:A:316:PRO:HD3	1:B:7:ILE:O	2.15	0.46
1:C:267:LYS:H	1:C:267:LYS:HD2	1.80	0.46
1:D:30:SER:H	1:D:34:LYS:HD3	1.80	0.46
1:A:168:THR:HG23	1:A:169:PRO:HD2	1.96	0.46
1:D:93:ARG:NH2	1:D:106:PHE:CE1	2.73	0.46
1:A:107:ARG:HG2	1:A:107:ARG:NH2	2.29	0.46
1:A:11:ILE:C	1:A:11:ILE:HD12	2.35	0.46
1:D:103:PRO:HG2	1:D:104:TYR:CD2	2.50	0.46
1:D:173:ARG:C	1:D:180:ILE:HD11	2.35	0.46
1:C:128:TRP:CE2	1:C:199:SER:HB2	2.51	0.46
1:D:271:GLN:O	1:D:272:ILE:HD13	2.16	0.46
1:C:115:ASN:H	1:C:120:ASN:HB3	1.81	0.46
1:C:78:THR:OG1	1:C:297:TYR:HB2	2.15	0.46
1:D:95:TRP:CH2	1:D:169:PRO:HD3	2.50	0.46
1:A:93:ARG:NH2	1:A:106:PHE:HE1	2.13	0.46
1:C:144:ILE:O	1:C:146:SER:N	2.49	0.46
1:B:254:ASP:CA	1:B:325:THR:HG22	2.36	0.46
1:B:12:VAL:HG23	1:B:12:VAL:O	2.16	0.46
1:B:65:VAL:HG23	2:B:337:CL:CL	2.53	0.46
1:C:201:ASN:O	1:C:250:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:HG3	1:B:10:ALA:HB2	1.98	0.45
1:D:253:LEU:C	1:D:325:THR:HG23	2.36	0.45
1:D:66:LEU:HD11	3:D:410:HOH:O	2.16	0.45
1:B:7:ILE:CG2	1:B:8:TYR:N	2.79	0.45
1:C:133:CYS:SG	1:C:136:VAL:HG13	2.57	0.45
1:B:100:TYR:O	1:B:103:PRO:HG3	2.15	0.45
1:C:95:TRP:HB3	1:C:120:ASN:OD1	2.17	0.45
1:B:324:GLN:NE2	1:B:324:GLN:HA	2.31	0.45
1:C:324:GLN:HA	1:C:324:GLN:NE2	2.31	0.45
1:D:150:LYS:HG2	1:D:154:LEU:HD11	1.99	0.45
1:D:261:ALA:O	1:D:266:ASN:ND2	2.50	0.45
1:A:211:PRO:HB3	1:A:223:TRP:CE2	2.51	0.45
1:B:150:LYS:O	1:B:154:LEU:HD23	2.16	0.45
1:C:140:GLY:HA2	3:C:391:HOH:O	2.17	0.45
1:C:165:ARG:CZ	1:C:167:MET:SD	3.05	0.45
1:D:156:LEU:C	1:D:158:GLY:H	2.20	0.45
1:D:228:ASN:HD21	1:D:231:TRP:H	1.65	0.45
1:D:140:GLY:N	1:D:160:TRP:CZ2	2.83	0.45
1:A:128:TRP:CE2	1:A:199:SER:HB2	2.52	0.45
1:C:11:ILE:HD11	1:D:312:MET:HB2	1.99	0.45
1:C:39:ILE:HD11	1:C:272:ILE:HD12	1.99	0.45
1:D:107:ARG:HG2	1:D:159:LYS:CE	2.47	0.45
1:C:113:VAL:CG2	1:C:208:ILE:HD13	2.46	0.45
1:C:95:TRP:CH2	1:C:169:PRO:HD3	2.52	0.44
1:D:61:PRO:HA	3:D:391:HOH:O	2.16	0.44
1:B:152:GLU:O	1:B:154:LEU:N	2.50	0.44
1:B:281:ALA:HA	1:B:303:MET:HB2	1.99	0.44
1:D:195:PRO:HG2	1:D:198:VAL:HG23	1.99	0.44
1:D:29:GLY:HA3	1:D:34:LYS:CD	2.45	0.44
1:C:38:PHE:O	1:C:274:ILE:HA	2.18	0.44
1:D:292:ALA:HB1	1:D:297:TYR:CE2	2.53	0.44
1:C:113:VAL:HG21	1:C:208:ILE:HD13	2.00	0.43
1:D:298:ASP:OD2	1:D:300:GLU:HG2	2.18	0.43
1:D:37:ILE:HD13	1:D:276:THR:HG22	1.99	0.43
1:A:287:ASP:HB3	1:A:288:PRO:HD2	2.00	0.43
1:C:144:ILE:O	1:C:144:ILE:HG22	2.18	0.43
1:C:274:ILE:HD11	1:C:330:ILE:HD12	2.00	0.43
1:C:308:GLU:HG3	1:D:240:TYR:CE2	2.53	0.43
1:B:164:ALA:O	1:B:165:ARG:O	2.37	0.43
1:B:75:MET:HE3	1:B:299:PRO:HA	2.01	0.43
1:C:43:ARG:HD2	3:C:387:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:HA	1:B:268:GLY:O	2.18	0.43
1:B:66:LEU:O	1:B:69:THR:HB	2.18	0.43
1:C:46:PRO:HB3	1:C:51:GLU:OE1	2.18	0.43
1:B:8:TYR:O	1:B:9:ARG:HD2	2.19	0.43
1:C:231:TRP:HA	1:C:234:ASP:OD2	2.18	0.43
1:C:50:ASN:HD22	1:C:50:ASN:N	1.96	0.43
1:A:139:THR:HG23	1:A:139:THR:O	2.19	0.43
1:B:51:GLU:HG3	1:B:52:ASN:N	2.33	0.43
1:C:213:PRO:HD2	2:C:337:CL:CL	2.56	0.43
1:C:41:PHE:HA	1:C:271:GLN:O	2.18	0.43
1:C:39:ILE:O	1:C:39:ILE:HG23	2.18	0.43
1:D:156:LEU:O	1:D:158:GLY:N	2.52	0.43
1:A:221:THR:HG22	3:A:466:HOH:O	2.18	0.43
1:B:267:LYS:HD3	1:B:267:LYS:N	2.34	0.43
1:B:106:PHE:C	1:B:107:ARG:HG3	2.38	0.43
1:B:105:THR:CG2	1:B:165:ARG:HG2	2.49	0.43
1:B:197:ASP:OD1	1:B:198:VAL:HG23	2.19	0.43
1:D:107:ARG:NH2	1:D:107:ARG:HG2	2.34	0.43
1:D:40:THR:CG2	1:D:78:THR:HG22	2.43	0.43
1:B:253:LEU:O	1:B:325:THR:HA	2.19	0.42
1:B:279:LEU:CD1	1:B:289:ASN:HD22	2.32	0.42
1:D:7:ILE:C	1:D:8:TYR:HD2	2.22	0.42
1:B:195:PRO:HA	1:B:196:PRO:HD3	1.97	0.42
1:C:132:ARG:NH2	1:C:132:ARG:HG3	2.34	0.42
1:C:276:THR:HG21	1:D:19:GLU:OE1	2.19	0.42
1:C:66:LEU:HD12	1:C:66:LEU:O	2.19	0.42
1:D:150:LYS:HG3	1:D:160:TRP:CD2	2.55	0.42
1:C:274:ILE:HD11	1:C:330:ILE:CD1	2.49	0.42
1:D:150:LYS:O	1:D:154:LEU:HG	2.19	0.42
1:C:150:LYS:O	1:C:153:CYS:N	2.53	0.42
1:C:178:GLY:O	1:C:189:GLU:HA	2.19	0.42
1:C:229:LEU:HA	1:C:229:LEU:HD23	1.87	0.42
1:B:226:GLU:HG2	1:B:227:ASP:N	2.35	0.42
1:D:107:ARG:HB2	1:D:110:ASP:OD1	2.19	0.42
1:B:175:ASP:C	1:B:177:GLU:H	2.22	0.42
1:B:255:SER:HA	1:B:258:PHE:CE2	2.54	0.42
1:B:80:LYS:HD2	1:B:294:LYS:O	2.19	0.42
1:C:211:PRO:HB3	1:C:223:TRP:CE2	2.54	0.42
1:A:150:LYS:HA	1:A:160:TRP:CE3	2.55	0.42
1:B:150:LYS:N	1:B:150:LYS:HD2	2.34	0.42
1:A:333:THR:HB	1:D:145:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HB	1:A:137:PRO:HD2	2.02	0.42
1:A:282:LYS:HD3	1:A:303:MET:HE3	2.00	0.42
1:B:298:ASP:O	1:B:300:GLU:N	2.53	0.42
1:B:7:ILE:CG2	1:B:8:TYR:H	2.31	0.42
1:C:135:ASP:C	1:C:136:VAL:HG22	2.40	0.42
1:C:254:ASP:CG	1:C:256:VAL:HG12	2.40	0.42
1:D:142:CYS:SG	1:D:143:SER:N	2.92	0.42
1:C:294:LYS:HG3	1:C:297:TYR:OH	2.20	0.41
1:C:233:GLN:HE22	1:D:305:HIS:CB	2.33	0.41
1:B:324:GLN:HE21	1:B:324:GLN:CA	2.27	0.41
1:B:120:ASN:HD22	1:B:120:ASN:HA	1.67	0.41
1:B:15:LYS:HB2	1:B:15:LYS:HE3	1.91	0.41
1:A:147:LEU:HD11	1:A:156:LEU:HD12	2.02	0.41
1:B:257:TYR:O	1:B:258:PHE:HB3	2.21	0.41
1:C:180:ILE:C	1:C:182:PRO:HD3	2.40	0.41
1:C:219:ASP:N	1:C:220:PRO:HD3	2.36	0.41
1:D:107:ARG:HB3	1:D:159:LYS:NZ	2.35	0.41
1:A:64:SER:HB2	2:A:337:CL:CL	2.58	0.41
1:B:61:PRO:HD3	1:B:314:ASN:HD22	1.84	0.41
1:A:311:TYR:CD2	1:A:332:PHE:HE2	2.38	0.41
1:A:95:TRP:CE3	1:A:169:PRO:HB3	2.55	0.41
1:C:166:SER:HA	1:C:186:TYR:CE1	2.56	0.41
1:C:319:ILE:N	1:C:319:ILE:CD1	2.80	0.41
1:C:320:MET:HB3	3:C:345:HOH:O	2.21	0.41
1:A:132:ARG:NH2	1:A:132:ARG:HG3	2.33	0.41
1:D:27:SER:O	1:D:35:ASN:N	2.52	0.41
1:D:196:PRO:HD2	3:D:384:HOH:O	2.21	0.41
1:D:318:ILE:HG22	1:D:318:ILE:O	2.20	0.41
1:B:12:VAL:HG21	3:B:376:HOH:O	2.21	0.41
1:B:303:MET:HG3	1:B:306:SER:HB3	2.01	0.41
1:D:228:ASN:ND2	1:D:231:TRP:H	2.19	0.41
1:C:233:GLN:HE22	1:D:305:HIS:HB3	1.86	0.41
1:B:37:ILE:CG2	1:B:81:VAL:HB	2.41	0.41
1:C:11:ILE:HD12	1:C:11:ILE:C	2.40	0.41
1:D:72:TRP:CZ3	1:D:304:ARG:HA	2.56	0.41
1:B:107:ARG:HH11	1:B:159:LYS:CD	2.23	0.40
1:B:168:THR:HA	1:B:169:PRO:HD3	1.92	0.40
1:B:60:TYR:HA	1:B:60:TYR:HD2	1.74	0.40
1:D:175:ASP:C	1:D:177:GLU:N	2.73	0.40
1:B:176:ALA:O	1:B:229:LEU:HD12	2.21	0.40
1:B:51:GLU:CG	1:B:52:ASN:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:O	1:C:160:TRP:HA	2.21	0.40
1:C:9:ARG:HD2	1:D:58:PRO:O	2.22	0.40
1:B:298:ASP:OD1	1:B:299:PRO:HD2	2.21	0.40
1:B:266:ASN:ND2	1:B:320:MET:H	2.18	0.40
1:C:330:ILE:HG22	1:C:331:LEU:N	2.37	0.40
1:D:174:GLY:HA3	1:D:180:ILE:HG12	2.03	0.40
1:D:22:LEU:HG	1:D:26:ASN:ND2	2.36	0.40
1:D:39:ILE:HG22	1:D:79:VAL:O	2.22	0.40
1:A:73:THR:HA	1:A:304:ARG:NH1	2.36	0.40
1:D:270:ARG:HG3	1:D:270:ARG:HH11	1.86	0.40
1:D:226:GLU:N	1:D:226:GLU:OE1	2.52	0.40
1:D:242:VAL:O	1:D:243:LYS:HB2	2.21	0.40
1:D:286:ASN:HB2	3:D:372:HOH:O	2.22	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	326/334 (98%)	301 (92%)	23 (7%)	2 (1%)	25	29
1	B	326/334 (98%)	271 (83%)	41 (13%)	14 (4%)	2	1
1	C	326/334 (98%)	293 (90%)	28 (9%)	5 (2%)	10	9
1	D	326/334 (98%)	293 (90%)	28 (9%)	5 (2%)	10	9
All	All	1304/1336 (98%)	1158 (89%)	120 (9%)	26 (2%)	7	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	GLU
1	B	144	ILE

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Mol	Chain	Res	Type
1	B	149	ASP
1	B	165	ARG
1	B	266	ASN
1	C	145	ALA
1	C	146	SER
1	A	98	THR
1	B	121	ALA
1	B	142	CYS
1	B	322	MET
1	C	133	CYS
1	D	146	SER
1	D	157	GLY
1	A	264	PRO
1	B	43	ARG
1	B	74	HIS
1	B	162	PRO
1	B	264	PRO
1	C	157	GLY
1	D	147	LEU
1	B	281	ALA
1	D	54	VAL
1	D	121	ALA
1	B	299	PRO
1	C	182	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/295 (98%)	276 (96%)	13 (4%)	27	36
1	B	289/295 (98%)	269 (93%)	20 (7%)	15	18
1	C	289/295 (98%)	274 (95%)	15 (5%)	23	30
1	D	289/295 (98%)	275 (95%)	14 (5%)	25	33
All	All	1156/1180 (98%)	1094 (95%)	62 (5%)	22	28

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PHE
1	A	45	GLU
1	A	50	ASN
1	A	70	ASP
1	A	107	ARG
1	A	161	THR
1	A	168	THR
1	A	205	ASN
1	A	264	PRO
1	A	295	ASP
1	A	305	HIS
1	A	315	ARG
1	A	319	ILE
1	B	9	ARG
1	B	16	PHE
1	B	37	ILE
1	B	39	ILE
1	B	52	ASN
1	B	60	TYR
1	B	62	THR
1	B	66	LEU
1	B	75	MET
1	B	120	ASN
1	B	168	THR
1	B	205	ASN
1	B	233	GLN
1	B	257	TYR
1	B	264	PRO
1	B	285	PRO
1	B	291	LYS
1	B	319	ILE
1	B	324	GLN
1	B	326	GLU
1	C	15	LYS
1	C	37	ILE
1	C	39	ILE
1	C	50	ASN
1	C	136	VAL
1	C	141	MET
1	C	205	ASN
1	C	218	GLU
1	C	233	GLN

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Mol	Chain	Res	Type
1	C	286	ASN
1	C	291	LYS
1	C	300	GLU
1	C	315	ARG
1	C	319	ILE
1	C	320	MET
1	D	7	ILE
1	D	16	PHE
1	D	39	ILE
1	D	50	ASN
1	D	107	ARG
1	D	110	ASP
1	D	156	LEU
1	D	161	THR
1	D	165	ARG
1	D	168	THR
1	D	222	ARG
1	D	229	LEU
1	D	233	GLN
1	D	273	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	52	ASN
1	A	205	ASN
1	A	232	GLN
1	A	233	GLN
1	A	324	GLN
1	B	50	ASN
1	B	120	ASN
1	B	201	ASN
1	B	233	GLN
1	B	289	ASN
1	B	324	GLN
1	B	329	ASN
1	C	50	ASN
1	C	205	ASN
1	C	233	GLN
1	C	286	ASN
1	C	324	GLN

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Mol	Chain	Res	Type
1	D	50	ASN
1	D	228	ASN
1	D	232	GLN
1	D	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

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.

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	328/334 (98%)	0.22	8 (2%) 59 54	19, 34, 53, 89	0
1	B	328/334 (98%)	1.10	76 (23%) 0 0	20, 54, 96, 100	0
1	C	328/334 (98%)	0.46	30 (9%) 9 6	14, 35, 78, 90	0
1	D	328/334 (98%)	0.51	41 (12%) 3 2	17, 41, 83, 89	0
All	All	1312/1336 (98%)	0.57	155 (11%) 4 3	14, 39, 85, 100	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	LEU	7.1
1	B	154	LEU	7.0
1	B	261	ALA	6.5
1	C	160	TRP	6.0
1	B	257	TYR	5.8
1	B	149	ASP	5.7
1	B	156	LEU	5.7
1	B	54	VAL	5.6
1	D	106	PHE	5.4
1	C	145	ALA	5.4
1	B	259	PRO	5.3
1	B	160	TRP	5.3
1	A	7	ILE	4.9
1	B	47	TRP	4.8
1	B	321	ALA	4.8
1	B	55	GLY	4.7
1	A	8	TYR	4.7
1	B	164	ALA	4.6
1	B	262	ALA	4.6
1	C	157	GLY	4.6
1	B	32	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	60	TYR	4.5
1	B	263	LEU	4.5
1	B	283	ALA	4.4
1	D	146	SER	4.4
1	B	253	LEU	4.4
1	B	302	LEU	4.4
1	B	319	ILE	4.4
1	B	269	PHE	4.0
1	B	284	HIS	4.0
1	C	164	ALA	4.0
1	B	33	ASP	3.9
1	B	78	THR	3.8
1	B	296	TYR	3.8
1	B	265	GLY	3.7
1	B	144	ILE	3.7
1	C	158	GLY	3.7
1	D	164	ALA	3.7
1	C	159	LYS	3.6
1	B	268	GLY	3.6
1	D	145	ALA	3.5
1	D	321	ALA	3.5
1	B	290	VAL	3.5
1	D	258	PHE	3.5
1	B	147	LEU	3.5
1	C	144	ILE	3.5
1	B	256	VAL	3.4
1	B	157	GLY	3.4
1	B	286	ASN	3.4
1	B	56	PHE	3.4
1	C	141	MET	3.3
1	D	159	LYS	3.3
1	B	258	PHE	3.3
1	B	159	LYS	3.3
1	B	292	ALA	3.3
1	B	255	SER	3.3
1	B	79	VAL	3.2
1	B	138	ASP	3.2
1	B	318	ILE	3.2
1	B	320	MET	3.2
1	B	57	ALA	3.2
1	D	105	THR	3.1
1	C	156	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	158	GLY	3.1
1	B	264	PRO	3.0
1	C	148	THR	3.0
1	D	182	PRO	3.0
1	B	260	GLU	3.0
1	B	324	GLN	3.0
1	D	55	GLY	3.0
1	B	145	ALA	2.9
1	C	33	ASP	2.9
1	D	152	GLU	2.9
1	C	32	PRO	2.9
1	C	147	LEU	2.9
1	C	262	ALA	2.9
1	D	156	LEU	2.9
1	D	136	VAL	2.9
1	D	324	GLN	2.9
1	D	322	MET	2.8
1	B	153	CYS	2.8
1	D	263	LEU	2.8
1	D	160	TRP	2.8
1	B	254	ASP	2.8
1	D	162	PRO	2.8
1	C	150	LYS	2.7
1	B	288	PRO	2.7
1	C	105	THR	2.7
1	D	56	PHE	2.7
1	C	163	SER	2.6
1	D	98	THR	2.6
1	D	261	ALA	2.6
1	D	264	PRO	2.6
1	C	143	SER	2.6
1	D	134	LEU	2.6
1	A	138	ASP	2.6
1	B	165	ARG	2.6
1	D	108	ILE	2.6
1	C	137	PRO	2.5
1	B	322	MET	2.5
1	B	267	LYS	2.5
1	B	315	ARG	2.5
1	A	164	ALA	2.5
1	D	32	PRO	2.5
1	A	236	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	135	ASP	2.5
1	C	176	ALA	2.5
1	A	104	TYR	2.5
1	D	138	ASP	2.4
1	B	148	THR	2.4
1	D	256	VAL	2.4
1	C	257	TYR	2.4
1	B	151	ASP	2.4
1	C	138	ASP	2.4
1	D	155	LYS	2.4
1	A	322	MET	2.4
1	B	155	LYS	2.4
1	B	50	ASN	2.4
1	D	183	GLY	2.3
1	C	162	PRO	2.3
1	D	157	GLY	2.3
1	B	285	PRO	2.3
1	B	293	GLU	2.3
1	B	142	CYS	2.3
1	B	162	PRO	2.3
1	B	150	LYS	2.3
1	B	136	VAL	2.3
1	B	287	ASP	2.3
1	D	161	THR	2.3
1	B	252	TYR	2.3
1	D	257	TYR	2.3
1	D	142	CYS	2.3
1	B	106	PHE	2.2
1	C	177	GLU	2.2
1	C	155	LYS	2.2
1	D	187	VAL	2.2
1	B	289	ASN	2.2
1	D	147	LEU	2.2
1	B	141	MET	2.1
1	D	33	ASP	2.1
1	C	165	ARG	2.1
1	B	266	ASN	2.1
1	D	316	PRO	2.1
1	D	102	ASP	2.1
1	C	322	MET	2.1
1	B	41	PHE	2.1
1	D	167	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASP	2.1
1	D	296	TYR	2.1
1	D	154	LEU	2.1
1	B	303	MET	2.0
1	A	10	ALA	2.0
1	B	168	THR	2.0
1	B	187	VAL	2.0
1	C	146	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	CL	C	342	1/1	0.39	0.83	120,120,120,120	0
2	CL	A	344	1/1	0.70	0.62	104,104,104,104	0
2	CL	B	338	1/1	0.73	0.24	85,85,85,85	0
2	CL	D	336	1/1	0.74	0.15	62,62,62,62	0
2	CL	B	340	1/1	0.80	0.16	61,61,61,61	0
2	CL	B	337	1/1	0.81	0.32	84,84,84,84	0
2	CL	A	339	1/1	0.81	0.21	69,69,69,69	0
2	CL	B	339	1/1	0.82	0.11	76,76,76,76	0
2	CL	C	339	1/1	0.82	0.14	54,54,54,54	0
2	CL	C	338	1/1	0.85	0.25	85,85,85,85	0
2	CL	D	340	1/1	0.86	0.11	65,65,65,65	0
2	CL	A	336	1/1	0.86	0.14	51,51,51,51	0
2	CL	A	340	1/1	0.87	0.12	61,61,61,61	0
2	CL	A	337	1/1	0.88	0.17	71,71,71,71	0
2	CL	B	336	1/1	0.89	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	C	335	1/1	0.90	0.35	67,67,67,67	0
2	CL	C	336	1/1	0.91	0.17	53,53,53,53	0
2	CL	A	335	1/1	0.92	0.11	57,57,57,57	0
2	CL	D	335	1/1	0.93	0.12	45,45,45,45	0
2	CL	D	338	1/1	0.94	0.15	72,72,72,72	0
2	CL	D	341	1/1	0.94	0.13	59,59,59,59	0
2	CL	C	340	1/1	0.94	0.16	55,55,55,55	0
2	CL	D	342	1/1	0.94	0.06	62,62,62,62	0
2	CL	D	339	1/1	0.95	0.34	82,82,82,82	0
2	CL	A	338	1/1	0.95	0.09	64,64,64,64	0
2	CL	A	343	1/1	0.95	0.22	62,62,62,62	0
2	CL	A	341	1/1	0.95	0.10	46,46,46,46	0
2	CL	B	335	1/1	0.95	0.09	45,45,45,45	0
2	CL	A	342	1/1	0.97	0.08	53,53,53,53	0
2	CL	C	341	1/1	0.97	0.08	44,44,44,44	0
2	CL	C	337	1/1	0.97	0.17	54,54,54,54	0
2	CL	D	337	1/1	0.99	0.20	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.