



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:53 PM UTC

PDB ID : 3ENH / pdb_00003enh
Title : Crystal structure of Cgi121/Bud32/Kae1 complex
Authors : Neculai, D.
Deposited on : 2008-09-25
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

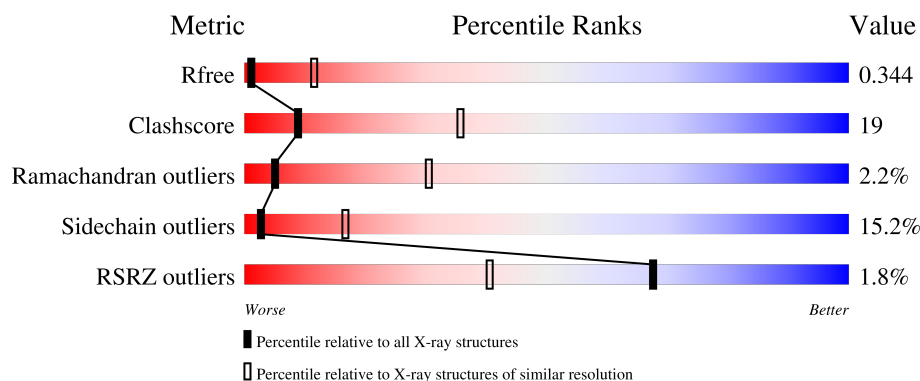
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	540	2% 49% 35% 7% 8%
1	B	540	% 52% 32% 6% 10%
2	C	150	% 55% 29% 7% 8%
2	D	150	% 52% 31% 9% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	A	5769	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10142 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 Putative O-sialoglycoprotein endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3926	2509	661	736	20			
1	B	485	Total	C	N	O	S	0	0	0
			3856	2466	643	726	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q58530
A	-3	ALA	-	expression tag	UNP Q58530
A	-2	MET	-	expression tag	UNP Q58530
A	-1	ASP	-	expression tag	UNP Q58530
A	0	PRO	-	expression tag	UNP Q58530
B	-4	GLY	-	expression tag	UNP Q58530
B	-3	ALA	-	expression tag	UNP Q58530
B	-2	MET	-	expression tag	UNP Q58530
B	-1	ASP	-	expression tag	UNP Q58530
B	0	PRO	-	expression tag	UNP Q58530

- Molecule 2 is a protein called Uncharacterized protein MJ0187.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1108	708	196	200	4			
2	D	138	Total	C	N	O	S	0	0	0
			1108	708	196	200	4			

There are 10 discrepancies between the modelled and reference sequences:

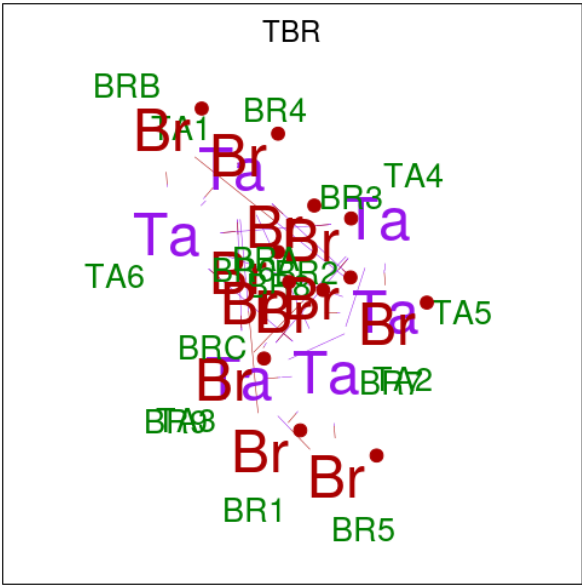
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP Q57646
C	2	ALA	-	expression tag	UNP Q57646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	expression tag	UNP Q57646
C	4	ASP	-	expression tag	UNP Q57646
C	5	PRO	-	expression tag	UNP Q57646
D	1	GLY	-	expression tag	UNP Q57646
D	2	ALA	-	expression tag	UNP Q57646
D	3	MET	-	expression tag	UNP Q57646
D	4	ASP	-	expression tag	UNP Q57646
D	5	PRO	-	expression tag	UNP Q57646

- Molecule 3 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).

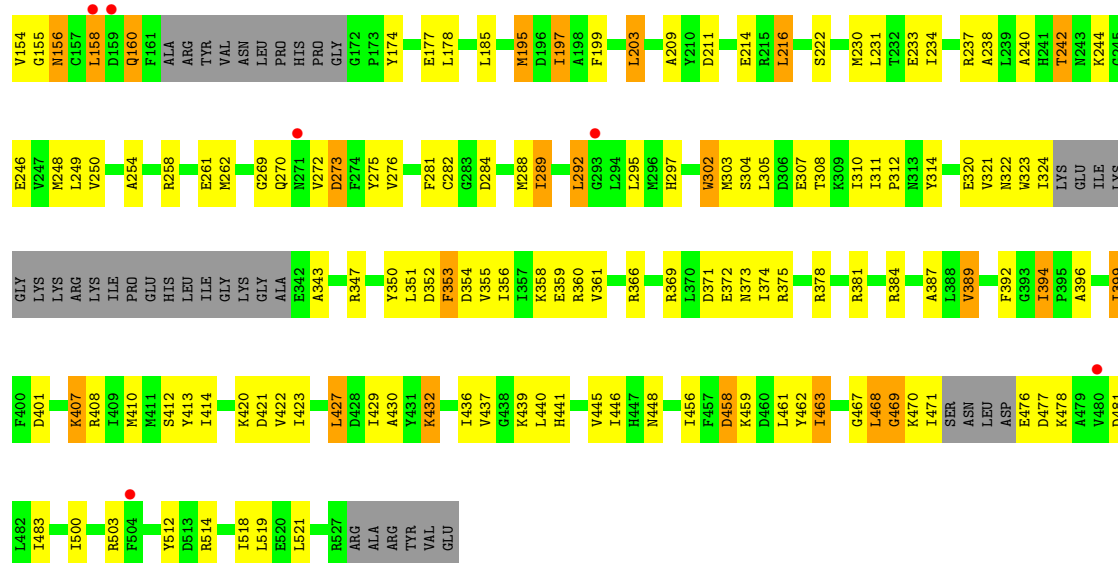


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		

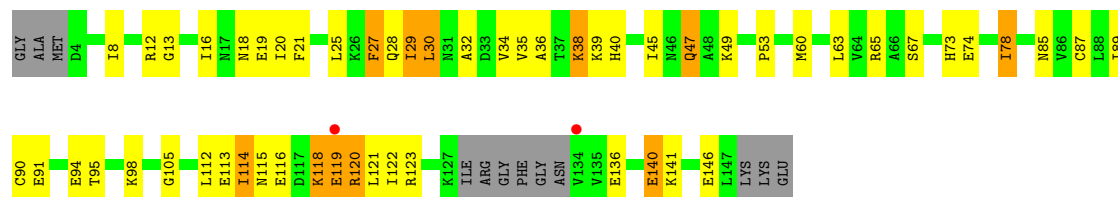
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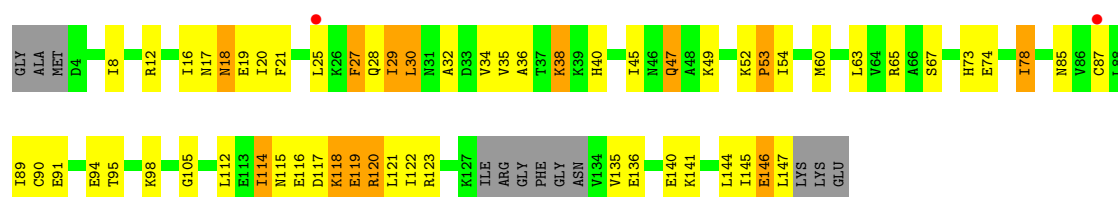
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Br	Ta		
3	B	1	18	12	6	0	0



• Molecule 2: Uncharacterized protein MJ0187



• Molecule 2: Uncharacterized protein MJ0187



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.99Å 106.91Å 209.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 3.60 94.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (94.92-3.60) 100.0 (94.92-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.271 , 0.324 0.287 , 0.344	Depositor DCC
R_{free} test set	1052 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	146.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 157.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10142	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: TBR

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	0.47	0/3994	0.85	0/5387
1	B	0.45	0/3921	0.84	2/5284 (0.0%)
2	C	0.52	0/1119	0.93	0/1499
2	D	0.52	0/1119	0.92	0/1499
All	All	0.47	0/10153	0.87	2/13669 (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	B	269	GLY	N-CA-C	-5.83	106.56	115.66
1	B	273	ASP	N-CA-C	5.77	118.90	108.69

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	3926	0	3959	177	0
1	B	3856	0	3887	141	0
2	C	1108	0	1168	31	0
2	D	1108	0	1168	36	0
3	A	72	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	72	0	0	5	0
All	All	10142	0	10182	377	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 19.

All (377) 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:A:11:GLU:OE2	3:A:5769:TBR:BR5	2.09	1.25
2:C:114:ILE:HD11	2:C:119:GLU:HB3	1.33	1.09
2:D:114:ILE:HD11	2:D:119:GLU:HB3	1.35	1.08
1:A:394:ILE:HD12	1:A:436:ILE:HB	1.47	0.96
1:B:394:ILE:HD12	1:B:436:ILE:HB	1.47	0.95
1:B:133:THR:HG22	1:B:153:ALA:HA	1.57	0.87
1:B:258:ARG:HH12	1:B:262:MET:HB3	1.40	0.86
1:A:133:THR:HG22	1:A:153:ALA:HA	1.57	0.85
1:A:159:ASP:HB3	3:A:5769:TBR:BRB	2.32	0.84
1:A:104:VAL:HG21	1:A:289:ILE:HB	1.57	0.84
2:D:27:PHE:CE1	2:D:95:THR:HB	2.13	0.84
1:B:56:ILE:HD11	1:B:93:LEU:HD21	1.61	0.83
1:A:384:ARG:HG3	2:D:147:LEU:HD22	1.61	0.83
1:A:56:ILE:HD11	1:A:93:LEU:HD21	1.64	0.80
2:C:27:PHE:CE1	2:C:95:THR:HB	2.16	0.80
1:B:113:ILE:HG12	1:B:288:MET:HB2	1.63	0.80
1:A:154:VAL:HG21	1:A:231:LEU:HD11	1.65	0.78
1:A:11:GLU:CD	3:A:5769:TBR:BR1	2.83	0.77
1:B:351:LEU:HG	2:C:39:LYS:HG3	1.67	0.77
1:A:159:ASP:OD2	3:A:5769:TBR:BR3	2.58	0.77
1:A:160:GLN:HE21	1:A:203:LEU:HD21	1.49	0.76
1:B:113:ILE:HG12	1:B:288:MET:CB	2.16	0.76
2:D:12:ARG:O	2:D:105:GLY:HA3	1.87	0.74
2:C:12:ARG:O	2:C:105:GLY:HA3	1.89	0.73
1:A:387:ALA:HB2	1:A:399:ILE:HD11	1.69	0.73
1:A:3:CYS:HB2	1:A:70:LEU:HB3	1.71	0.72
1:B:3:CYS:HB2	1:B:70:LEU:HB3	1.71	0.72
1:A:355:VAL:HG12	1:A:412:SER:HA	1.72	0.72
1:A:384:ARG:HG3	2:D:147:LEU:CD2	2.20	0.71
1:B:195:MET:HG2	1:B:237:ARG:HE	1.54	0.71
1:B:352:ASP:HB2	2:C:39:LYS:HE2	1.73	0.70
1:B:154:VAL:HG21	1:B:231:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD3	1:A:169:HIS:HE1	1.55	0.70
1:B:355:VAL:HG12	1:B:412:SER:HA	1.74	0.69
1:B:456:ILE:HD11	1:B:462:TYR:HB2	1.73	0.69
1:A:456:ILE:HD11	1:A:462:TYR:HB2	1.74	0.69
1:B:270:GLN:HG2	1:B:272:VAL:HG22	1.75	0.68
1:B:387:ALA:HB2	1:B:399:ILE:HD11	1.74	0.68
1:A:1:MET:HB2	3:A:6769:TBR:BR6	2.48	0.68
1:A:124:LEU:HD11	1:A:238:ALA:HB1	1.75	0.68
1:A:315:ARG:NH1	1:A:317:ASP:HB2	2.07	0.68
1:A:77:PRO:HD3	1:A:314:TYR:HB3	1.75	0.68
1:A:427:LEU:HD22	1:A:503:ARG:HD3	1.74	0.68
1:A:297:HIS:CE1	3:A:6769:TBR:BR7	3.02	0.67
1:B:427:LEU:HD22	1:B:503:ARG:HD3	1.77	0.67
1:B:104:VAL:HB	1:B:292:LEU:HD12	1.75	0.67
1:B:7:GLU:HB2	1:B:289:ILE:CD1	2.23	0.67
1:A:106:HIS:HE1	1:A:284:ASP:HB3	1.60	0.66
1:B:238:ALA:O	1:B:242:THR:OG1	2.12	0.66
1:B:113:ILE:HD13	1:B:281:PHE:HB3	1.78	0.66
1:B:133:THR:CG2	1:B:153:ALA:HA	2.26	0.66
1:A:133:THR:CG2	1:A:153:ALA:HA	2.24	0.66
1:B:19:THR:HG23	1:B:25:LEU:HD21	1.78	0.65
1:B:130:GLY:HA2	1:B:155:GLY:HA3	1.78	0.65
1:A:3:CYS:HB3	1:A:294:LEU:HD23	1.78	0.64
1:A:355:VAL:HA	1:A:413:TYR:H	1.63	0.64
1:B:297:HIS:HE1	3:B:3769:TBR:BRB	2.35	0.64
2:D:36:ALA:HB3	2:D:40:HIS:HB2	1.79	0.64
1:A:134:GLN:HG3	1:A:136:ILE:HD11	1.80	0.63
1:B:134:GLN:HG3	1:B:136:ILE:HD11	1.79	0.63
2:C:36:ALA:HB3	2:C:40:HIS:HB2	1.79	0.63
1:A:130:GLY:HA2	1:A:155:GLY:HA3	1.81	0.63
1:A:19:THR:HG23	1:A:25:LEU:HD21	1.80	0.63
1:B:355:VAL:HA	1:B:413:TYR:H	1.63	0.62
1:A:231:LEU:O	1:A:234:ILE:HD13	1.99	0.62
2:C:28:GLN:NE2	2:C:63:LEU:HB2	2.15	0.61
1:A:159:ASP:OD2	3:A:5769:TBR:BR6	2.73	0.61
2:D:120:ARG:HD3	2:D:120:ARG:N	2.15	0.61
1:A:249:LEU:HB3	1:A:276:VAL:HG12	1.82	0.61
1:A:236:GLU:HG3	1:A:266:MET:HE3	1.82	0.61
1:A:2:ILE:HG22	1:A:19:THR:HA	1.83	0.60
1:A:259:LEU:O	1:A:263:LEU:HB2	2.01	0.60
1:B:139:VAL:HG21	1:B:146:PHE:HZ	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:120:ARG:HD3	2:C:120:ARG:N	2.18	0.59
1:B:2:ILE:HG22	1:B:19:THR:HA	1.84	0.59
1:A:168:PRO:HB2	1:A:174:TYR:HE2	1.67	0.59
1:B:7:GLU:HB2	1:B:289:ILE:HD11	1.83	0.59
1:A:159:ASP:CB	3:A:5769:TBR:BRB	3.03	0.59
1:A:138:TYR:CE1	1:A:321:VAL:HG21	2.38	0.58
2:D:32:ALA:HB3	2:D:85:ASN:HD22	1.69	0.58
1:A:162:ALA:HB2	1:A:175:ILE:HD11	1.85	0.58
1:B:74:SER:HB3	1:B:289:ILE:HG21	1.85	0.58
1:A:476:GLU:HG2	1:A:521:LEU:HD11	1.86	0.58
2:D:28:GLN:NE2	2:D:63:LEU:HB2	2.18	0.58
2:D:32:ALA:HA	2:D:35:VAL:HG12	1.85	0.58
1:A:222:SER:HA	1:A:225:GLU:HB2	1.86	0.57
1:A:315:ARG:H	1:A:318:MET:HE2	1.69	0.57
2:C:47:GLN:HG3	2:C:65:ARG:HH21	1.69	0.57
1:B:121:GLU:OE1	3:B:7769:TBR:BR8	2.77	0.57
1:A:242:THR:HB	1:A:244:LYS:HD3	1.86	0.57
2:D:38:LYS:HG3	2:D:112:LEU:HD13	1.86	0.57
1:A:441:HIS:HD2	1:A:478:LYS:HB3	1.68	0.57
1:B:141:LYS:O	1:B:321:VAL:HG22	2.04	0.56
2:C:115:ASN:H	2:C:118:LYS:HD3	1.69	0.56
1:A:112:GLU:HG3	1:A:292:LEU:HD13	1.88	0.56
1:B:360:ARG:HH12	1:B:378:ARG:CB	2.18	0.56
2:C:32:ALA:HB3	2:C:85:ASN:HD22	1.70	0.56
2:D:115:ASN:H	2:D:118:LYS:HD3	1.69	0.56
1:A:18:VAL:HG12	1:A:24:VAL:HA	1.88	0.56
1:A:105:ASN:ND2	1:A:108:ILE:H	2.03	0.56
1:B:112:GLU:HG3	1:B:292:LEU:HD23	1.86	0.56
1:B:476:GLU:HG2	1:B:521:LEU:HD11	1.87	0.56
1:B:105:ASN:HD22	1:B:108:ILE:H	1.52	0.56
1:A:11:GLU:OE2	3:A:5769:TBR:BR1	2.79	0.56
1:A:139:VAL:HG21	1:A:146:PHE:HZ	1.70	0.56
1:A:437:VAL:HA	1:A:440:LEU:HD12	1.87	0.56
2:C:45:ILE:O	2:C:49:LYS:HB2	2.06	0.56
1:A:387:ALA:CB	2:D:144:LEU:HD11	2.36	0.56
1:B:311:ILE:HB	1:B:314:TYR:HB2	1.87	0.56
1:A:369:ARG:O	1:A:373:ASN:HB2	2.06	0.56
1:B:369:ARG:O	1:B:373:ASN:HB2	2.06	0.56
2:D:27:PHE:HB3	2:D:90:CYS:HA	1.88	0.56
1:A:197:ILE:HD11	1:A:234:ILE:HD12	1.88	0.55
1:B:289:ILE:HD13	1:B:289:ILE:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:HB2	1:B:289:ILE:HD12	1.89	0.55
1:B:87:ALA:HB2	1:B:310:ILE:HG23	1.89	0.55
1:B:436:ILE:HA	1:B:439:LYS:HG3	1.89	0.55
1:B:441:HIS:HD2	1:B:478:LYS:HB3	1.72	0.55
1:B:105:ASN:ND2	1:B:108:ILE:H	2.05	0.55
1:B:94:SER:HB3	1:B:101:ILE:HG23	1.90	0.54
2:D:45:ILE:O	2:D:49:LYS:HB2	2.06	0.54
1:A:315:ARG:O	1:A:318:MET:HG2	2.06	0.54
1:A:105:ASN:HD22	1:A:108:ILE:H	1.53	0.54
1:B:429:ILE:HG23	1:B:461:LEU:HD11	1.90	0.54
1:B:185:LEU:HB2	1:B:369:ARG:NH1	2.23	0.54
2:D:47:GLN:HE21	2:D:47:GLN:HA	1.73	0.54
1:A:185:LEU:HB2	1:A:369:ARG:NH1	2.23	0.53
1:B:111:ILE:HG23	1:B:125:THR:HG21	1.90	0.53
2:C:38:LYS:HG3	2:C:112:LEU:HD13	1.88	0.53
1:A:110:HIS:CE1	1:A:288:MET:HE1	2.43	0.53
1:A:111:ILE:HG23	1:A:125:THR:HG21	1.90	0.53
2:C:27:PHE:HB3	2:C:90:CYS:HA	1.91	0.53
1:A:168:PRO:HB2	1:A:174:TYR:CE2	2.44	0.53
1:A:360:ARG:HH12	1:A:378:ARG:CB	2.21	0.53
1:A:74:SER:HB3	1:A:289:ILE:HG21	1.90	0.53
1:A:313:ASN:H	1:A:313:ASN:ND2	2.06	0.53
1:B:30:ILE:HD12	1:B:51:THR:HG23	1.91	0.53
1:A:185:LEU:HD22	1:A:222:SER:HB3	1.91	0.52
2:C:32:ALA:HA	2:C:35:VAL:HG12	1.92	0.52
1:A:94:SER:HB3	1:A:101:ILE:HG23	1.92	0.52
1:B:83:LEU:HD23	1:B:310:ILE:HB	1.92	0.52
1:B:117:THR:HG21	1:B:281:PHE:CD1	2.44	0.52
1:B:437:VAL:HA	1:B:440:LEU:HD12	1.91	0.51
1:A:163:ARG:CZ	3:A:5769:TBR:BR8	3.14	0.51
1:A:228:PHE:CD1	1:A:259:LEU:HD12	2.45	0.51
1:A:164:TYR:CD2	1:A:207:MET:HE2	2.45	0.51
1:B:310:ILE:HD12	1:B:312:PRO:HD3	1.93	0.51
1:B:119:GLU:HG3	1:B:275:TYR:HE1	1.75	0.51
2:C:87:CYS:HB3	2:C:112:LEU:CD2	2.41	0.51
1:A:204:THR:O	1:A:208:ARG:HG3	2.10	0.51
1:B:249:LEU:HG	1:B:254:ALA:HB1	1.92	0.51
1:B:389:VAL:O	1:B:394:ILE:HG23	2.11	0.51
2:C:47:GLN:HA	2:C:47:GLN:HE21	1.76	0.51
2:D:47:GLN:HG3	2:D:65:ARG:HH21	1.76	0.51
1:B:18:VAL:HG12	1:B:24:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HB	1:B:51:THR:HG21	1.93	0.50
1:A:113:ILE:HG12	1:A:288:MET:HA	1.94	0.50
1:B:366:ARG:HG3	1:B:371:ASP:HB2	1.94	0.50
1:A:429:ILE:HG23	1:A:461:LEU:HD11	1.94	0.50
1:A:436:ILE:HA	1:A:439:LYS:HG3	1.91	0.50
1:B:246:GLU:HA	1:B:273:ASP:HB3	1.93	0.50
1:B:347:ARG:HG2	1:B:356:ILE:HG22	1.94	0.50
1:B:360:ARG:HH12	1:B:378:ARG:HB2	1.76	0.50
1:A:11:GLU:HG2	3:A:5769:TBR:BR1	2.67	0.50
2:D:120:ARG:HD3	2:D:120:ARG:H	1.77	0.50
1:A:226:TYR:O	1:A:230:MET:HG2	2.11	0.49
1:B:297:HIS:CE1	3:B:3769:TBR:BRB	3.20	0.49
1:A:422:VAL:HG23	1:A:429:ILE:HD13	1.94	0.49
1:B:459:LYS:HE2	1:B:459:LYS:HA	1.93	0.49
1:B:272:VAL:HG23	1:B:273:ASP:N	2.27	0.49
1:B:399:ILE:O	2:C:140:GLU:HB2	2.11	0.49
2:C:16:ILE:HD11	2:C:29:ILE:HD11	1.94	0.49
2:D:16:ILE:HD11	2:D:29:ILE:HD11	1.93	0.49
1:B:156:ASN:C	1:B:156:ASN:HD22	2.19	0.49
1:A:267:CYS:HB2	1:A:272:VAL:HG23	1.94	0.49
1:A:18:VAL:HG23	1:A:294:LEU:HD21	1.95	0.49
1:B:414:ILE:HD11	1:B:458:ASP:HB2	1.94	0.49
1:A:104:VAL:CG2	1:A:289:ILE:HB	2.36	0.49
1:A:459:LYS:HA	1:A:459:LYS:HE2	1.94	0.49
1:B:149:THR:HG23	1:B:151:ASP:H	1.77	0.49
1:A:66:ASN:H	1:A:66:ASN:ND2	2.11	0.48
1:A:142:LYS:HB2	1:A:144:ARG:NH2	2.28	0.48
1:A:347:ARG:HG2	1:A:356:ILE:HG22	1.95	0.48
1:B:470:LYS:HG3	1:B:471:ILE:H	1.77	0.48
1:A:149:THR:HG23	1:A:151:ASP:H	1.78	0.48
1:A:384:ARG:HH12	1:A:470:LYS:HZ1	1.60	0.48
1:B:343:ALA:HA	1:B:361:VAL:HG12	1.95	0.48
2:D:87:CYS:HB3	2:D:112:LEU:CD2	2.43	0.48
1:A:343:ALA:HB1	1:A:360:ARG:HA	1.94	0.48
1:B:185:LEU:HB2	1:B:369:ARG:HH11	1.79	0.48
1:B:422:VAL:HG23	1:B:429:ILE:HD13	1.95	0.48
1:B:24:VAL:HG21	1:B:27:ASN:HB2	1.95	0.48
1:B:295:LEU:HD22	1:B:323:TRP:HB2	1.95	0.48
1:B:142:LYS:HB2	1:B:144:ARG:NH2	2.28	0.48
1:B:512:TYR:CZ	1:B:514:ARG:HB2	2.49	0.48
1:A:30:ILE:HD12	1:A:51:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:HG23	1:A:522:MET:SD	2.54	0.48
2:C:34:VAL:HG13	2:C:122:ILE:HG13	1.96	0.48
1:A:165:VAL:HG11	1:A:216:LEU:HD11	1.96	0.48
1:A:470:LYS:HG3	1:A:471:ILE:H	1.78	0.48
1:A:384:ARG:HH12	1:A:470:LYS:NZ	2.11	0.47
1:B:66:ASN:ND2	1:B:66:ASN:H	2.12	0.47
1:B:401:ASP:HB3	1:B:410:MET:HB3	1.96	0.47
1:B:423:ILE:HD11	1:B:430:ALA:HB2	1.96	0.47
1:B:195:MET:HG3	1:B:237:ARG:HH21	1.77	0.47
1:A:313:ASN:H	1:A:313:ASN:HD22	1.61	0.47
1:A:358:LYS:O	1:A:408:ARG:HA	2.14	0.47
1:A:106:HIS:CE1	1:A:284:ASP:HB3	2.47	0.47
2:C:120:ARG:HD3	2:C:120:ARG:H	1.79	0.47
2:D:47:GLN:HA	2:D:47:GLN:NE2	2.28	0.47
1:A:432:LYS:HB3	1:A:461:LEU:HD12	1.97	0.47
1:A:30:ILE:HB	1:A:51:THR:HG21	1.97	0.47
1:A:156:ASN:C	1:A:156:ASN:HD22	2.23	0.47
2:D:34:VAL:HG13	2:D:122:ILE:HG13	1.96	0.47
1:A:154:VAL:HG22	1:A:199:PHE:CZ	2.50	0.47
1:A:297:HIS:HE1	3:A:6769:TBR:BR8	2.53	0.47
1:A:423:ILE:HD11	1:A:430:ALA:HB2	1.97	0.47
1:A:185:LEU:HB2	1:A:369:ARG:HH11	1.80	0.47
1:A:381:ARG:HD3	1:A:470:LYS:HD2	1.96	0.47
1:B:137:ALA:HB1	1:B:244:LYS:HE3	1.97	0.47
1:B:231:LEU:O	1:B:234:ILE:HG13	2.14	0.47
1:A:355:VAL:HA	1:A:413:TYR:N	2.29	0.46
1:B:174:TYR:HA	1:B:177:GLU:HB2	1.96	0.46
1:B:321:VAL:HA	1:B:323:TRP:CZ3	2.49	0.46
1:A:343:ALA:HA	1:A:361:VAL:HG12	1.97	0.46
1:A:358:LYS:HB2	1:A:409:ILE:HG22	1.97	0.46
1:B:110:HIS:HB3	1:B:250:VAL:HG21	1.96	0.46
1:A:11:GLU:HB2	3:A:5769:TBR:BR5	2.70	0.46
1:B:103:GLY:H	1:B:303:MET:HG3	1.80	0.46
1:B:127:TYR:O	1:B:133:THR:HA	2.16	0.46
2:C:8:ILE:HG22	2:C:89:ILE:HG12	1.98	0.46
1:A:285:ASN:ND2	1:A:288:MET:HB2	2.30	0.46
1:A:315:ARG:O	1:A:317:ASP:N	2.49	0.46
2:D:67:SER:HB2	2:D:78:ILE:HD11	1.98	0.46
1:A:526:GLU:C	1:A:528:ARG:H	2.24	0.46
1:B:19:THR:OG1	1:B:23:GLU:HG2	2.16	0.45
1:B:343:ALA:HB1	1:B:360:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HA	1:A:111:ILE:HD12	1.97	0.45
1:A:232:THR:HG23	1:A:263:LEU:HD22	1.99	0.45
1:A:414:ILE:HD11	1:A:458:ASP:HB2	1.98	0.45
1:B:359:GLU:OE1	1:B:408:ARG:HB3	2.16	0.45
2:D:27:PHE:HB2	2:D:89:ILE:O	2.16	0.45
1:A:110:HIS:O	1:A:250:VAL:HG11	2.17	0.45
2:D:8:ILE:HG22	2:D:89:ILE:HG12	1.97	0.45
2:D:12:ARG:HD2	2:D:85:ASN:HB3	1.98	0.45
1:A:24:VAL:HG21	1:A:27:ASN:HB2	1.98	0.45
1:A:456:ILE:CD1	1:A:462:TYR:HB2	2.44	0.45
1:A:20:SER:HA	1:A:294:LEU:HD13	1.99	0.45
1:A:366:ARG:HG3	1:A:371:ASP:HB2	1.98	0.45
1:A:228:PHE:O	1:A:232:THR:OG1	2.34	0.45
1:A:360:ARG:HH12	1:A:378:ARG:HB2	1.82	0.45
1:A:389:VAL:O	1:A:394:ILE:HG23	2.17	0.45
1:B:109:ALA:O	1:B:113:ILE:HG13	2.16	0.45
2:C:47:GLN:HA	2:C:47:GLN:NE2	2.32	0.45
1:A:114:GLY:HA2	1:A:277:PRO:HG3	1.99	0.45
1:A:512:TYR:CZ	1:A:514:ARG:HB2	2.51	0.45
1:A:17:ILE:HD13	1:A:63:VAL:HG11	1.99	0.45
1:A:110:HIS:HE1	1:A:282:CYS:O	2.00	0.45
1:A:123:PRO:HA	1:A:246:GLU:HG3	1.98	0.45
1:B:209:ALA:O	1:B:214:GLU:HB2	2.17	0.45
1:A:11:GLU:CB	3:A:5769:TBR:BR5	3.20	0.45
1:A:109:ALA:O	1:A:113:ILE:HG13	2.17	0.44
1:A:189:PRO:HD3	1:A:205:ALA:CB	2.46	0.44
1:A:387:ALA:HB1	2:D:144:LEU:HD11	1.99	0.44
1:A:401:ASP:HB3	1:A:410:MET:HB3	1.97	0.44
1:B:355:VAL:HA	1:B:413:TYR:N	2.29	0.44
1:B:381:ARG:HD3	1:B:470:LYS:HD2	1.99	0.44
2:C:27:PHE:HB2	2:C:89:ILE:O	2.17	0.44
1:B:60:PHE:CD1	1:B:65:LYS:HG2	2.52	0.44
2:C:12:ARG:HD2	2:C:85:ASN:HB3	2.00	0.44
1:B:9:THR:HA	1:B:83:LEU:HD12	1.98	0.44
1:B:197:ILE:CG2	1:B:230:MET:HB3	2.48	0.44
1:A:60:PHE:CD1	1:A:65:LYS:HG2	2.52	0.44
1:B:125:THR:HG22	1:B:248:MET:HB3	2.00	0.44
1:B:154:VAL:HG22	1:B:199:PHE:CZ	2.53	0.44
1:B:139:VAL:HG21	1:B:146:PHE:CZ	2.50	0.44
1:B:353:PHE:CE2	2:C:136:GLU:HG2	2.53	0.44
1:A:76:GLY:HA2	1:A:314:TYR:HD1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:SER:HB2	2:C:78:ILE:HD11	1.99	0.44
1:A:448:ASN:ND2	1:A:469:GLY:HA2	2.33	0.43
1:A:514:ARG:HA	1:A:517:ILE:HD13	2.00	0.43
1:B:456:ILE:CD1	1:B:462:TYR:HB2	2.43	0.43
1:A:16:GLY:HA2	1:A:26:PHE:O	2.18	0.43
1:B:83:LEU:HD22	1:B:312:PRO:HA	1.99	0.43
1:B:436:ILE:HA	1:B:439:LYS:CG	2.48	0.43
1:A:362:LYS:HB2	1:A:371:ASP:OD2	2.17	0.43
1:B:358:LYS:O	1:B:408:ARG:HA	2.18	0.43
1:A:9:THR:HA	1:A:83:LEU:HD12	2.01	0.43
1:A:126:LEU:HD11	1:A:231:LEU:HD22	2.01	0.43
1:A:264:LYS:O	1:A:265:ALA:C	2.62	0.43
1:A:17:ILE:HG22	1:A:26:PHE:HB3	2.00	0.43
1:A:127:TYR:O	1:A:133:THR:HA	2.19	0.43
1:A:210:TYR:HA	1:A:219:ILE:HD13	2.01	0.43
1:B:178:LEU:HD13	1:B:216:LEU:HD13	2.00	0.43
1:A:359:GLU:OE1	1:A:408:ARG:HB3	2.19	0.43
1:A:480:VAL:O	1:A:484:VAL:HG23	2.19	0.43
2:C:113:GLU:H	2:C:113:GLU:HG2	1.70	0.43
1:A:436:ILE:HA	1:A:439:LYS:CG	2.49	0.43
1:B:394:ILE:CD1	1:B:436:ILE:HB	2.35	0.43
1:A:174:TYR:HA	1:A:177:GLU:HB2	2.00	0.42
1:B:356:ILE:HG23	1:B:413:TYR:HB2	2.01	0.42
1:B:448:ASN:HB2	1:B:468:LEU:HD12	2.01	0.42
1:A:11:GLU:CG	3:A:5769:TBR:BR1	3.22	0.42
1:A:315:ARG:HH11	1:A:315:ARG:HB3	1.84	0.42
1:B:17:ILE:HG22	1:B:26:PHE:HB3	2.01	0.42
1:A:448:ASN:HD22	1:A:469:GLY:HA2	1.84	0.42
1:B:17:ILE:HD13	1:B:63:VAL:HG11	2.02	0.42
1:B:17:ILE:HG21	1:B:63:VAL:HG11	2.02	0.42
1:B:108:ILE:HA	1:B:111:ILE:HD12	2.01	0.42
1:A:143:TYR:O	1:A:317:ASP:HA	2.20	0.42
1:B:123:PRO:HB2	1:B:248:MET:HB2	2.01	0.42
1:B:160:GLN:HB3	1:B:203:LEU:HD11	2.01	0.42
1:A:315:ARG:N	1:A:318:MET:HE2	2.33	0.42
1:A:351:LEU:HD12	1:A:351:LEU:HA	1.97	0.42
1:A:446:ILE:HD11	1:A:481:ASP:HB2	2.02	0.42
1:B:432:LYS:HB3	1:B:461:LEU:HD12	2.00	0.42
2:D:144:LEU:C	2:D:146:GLU:H	2.27	0.42
1:A:66:ASN:H	1:A:66:ASN:HD22	1.67	0.42
1:A:142:LYS:HG3	1:A:319:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HD11	1:A:411:MET:HE2	2.02	0.42
1:B:476:GLU:OE1	3:B:2769:TBR:BR9	2.93	0.42
1:A:531:TYR:O	1:A:532:VAL:C	2.62	0.42
1:A:133:THR:HG23	1:A:149:THR:HB	2.02	0.42
1:B:446:ILE:HD11	1:B:481:ASP:HB2	2.02	0.42
1:A:17:ILE:HG21	1:A:63:VAL:HG11	2.02	0.41
1:A:124:LEU:HD12	1:A:137:ALA:HB2	2.00	0.41
1:A:138:TYR:HB2	1:A:143:TYR:CE1	2.54	0.41
1:A:165:VAL:HG13	1:A:210:TYR:CZ	2.56	0.41
1:B:124:LEU:HD12	1:B:137:ALA:HB2	2.02	0.41
1:B:288:MET:HG3	1:B:289:ILE:N	2.35	0.41
2:D:52:LYS:HA	2:D:53:PRO:HD3	1.96	0.41
1:A:93:LEU:O	1:A:97:LEU:HB2	2.19	0.41
1:A:375:ARG:C	1:A:407:LYS:HG2	2.45	0.41
1:B:121:GLU:HB2	3:B:7769:TBR:BR4	2.75	0.41
2:C:28:GLN:HE22	2:C:63:LEU:HB2	1.85	0.41
2:D:34:VAL:HG12	2:D:34:VAL:O	2.20	0.41
1:A:105:ASN:HD21	1:A:107:CYS:HB2	1.85	0.41
1:A:124:LEU:HD11	1:A:238:ALA:CB	2.48	0.41
1:B:396:ALA:HB2	1:B:463:ILE:HD12	2.02	0.41
1:B:93:LEU:O	1:B:97:LEU:HB2	2.21	0.41
1:B:154:VAL:O	1:B:158:LEU:HB2	2.20	0.41
1:B:384:ARG:HH12	1:B:470:LYS:NZ	2.19	0.41
1:A:154:VAL:O	1:A:158:LEU:HB2	2.21	0.41
1:A:381:ARG:HD3	1:A:470:LYS:CD	2.51	0.41
1:A:445:VAL:HA	1:A:471:ILE:HG22	2.01	0.41
1:A:448:ASN:HB2	1:A:468:LEU:HD12	2.02	0.41
2:D:117:ASP:HA	2:D:120:ARG:NE	2.36	0.41
2:D:135:VAL:HG23	2:D:136:GLU:HG3	2.03	0.41
1:B:133:THR:HG23	1:B:149:THR:HB	2.02	0.41
1:A:356:ILE:HG23	1:A:413:TYR:HB2	2.03	0.41
1:B:185:LEU:HA	1:B:222:SER:OG	2.21	0.41
2:C:34:VAL:O	2:C:34:VAL:HG12	2.21	0.41
1:A:178:LEU:HD13	1:A:216:LEU:HD13	2.03	0.41
1:A:316:THR:C	1:A:318:MET:H	2.28	0.41
1:B:156:ASN:O	1:B:160:GLN:HB2	2.20	0.41
1:B:350:TYR:HB2	1:B:410:MET:SD	2.61	0.41
1:B:448:ASN:ND2	1:B:469:GLY:HA2	2.36	0.41
2:D:17:ASN:O	2:D:18:ASN:C	2.63	0.41
2:D:30:LEU:HD12	2:D:63:LEU:HD22	2.03	0.41
1:A:163:ARG:HD3	1:A:169:HIS:CE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ALA:HB1	1:B:123:PRO:HG3	2.03	0.41
1:B:375:ARG:C	1:B:407:LYS:HG2	2.46	0.41
1:B:445:VAL:HA	1:B:471:ILE:HG22	2.03	0.41
1:B:111:ILE:O	1:B:248:MET:HE1	2.20	0.40
1:B:142:LYS:HE2	1:B:320:GLU:HA	2.03	0.40
2:D:78:ILE:H	2:D:78:ILE:HG13	1.82	0.40
1:B:12:LYS:HB3	1:B:29:THR:CG2	2.51	0.40
1:B:128:VAL:HG23	1:B:254:ALA:HB2	2.03	0.40
1:A:76:GLY:HA2	1:A:314:TYR:HB2	2.03	0.40
1:A:176:GLU:HA	1:A:224:GLN:HE22	1.86	0.40
1:B:87:ALA:HB2	1:B:310:ILE:CG2	2.51	0.40
1:B:113:ILE:HG21	1:B:288:MET:HA	2.03	0.40
1:A:350:TYR:CG	1:A:351:LEU:N	2.87	0.40
2:D:54:ILE:HG22	2:D:65:ARG:HH11	1.86	0.40
1:A:394:ILE:CD1	1:A:436:ILE:HB	2.34	0.40
1:B:302:TRP:HZ3	1:B:304:SER:HA	1.85	0.40
2:C:30:LEU:HB2	2:C:87:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	487/540 (90%)	423 (87%)	57 (12%)	7 (1%)	9	38
1	B	475/540 (88%)	421 (89%)	50 (10%)	4 (1%)	16	49
2	C	134/150 (89%)	115 (86%)	11 (8%)	8 (6%)	1	13
2	D	134/150 (89%)	115 (86%)	11 (8%)	8 (6%)	1	13
All	All	1230/1380 (89%)	1074 (87%)	129 (10%)	27 (2%)	5	30

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	THR
1	B	240	ALA
2	D	21	PHE
1	A	467	GLY
2	C	21	PHE
2	C	25	LEU
2	D	25	LEU
1	A	256	ASN
1	B	467	GLY
2	C	19	GLU
2	D	18	ASN
2	D	19	GLU
2	D	119	GLU
1	A	172	GLY
2	C	18	ASN
2	C	119	GLU
1	A	279	LYS
1	B	469	GLY
1	A	141	LYS
1	A	469	GLY
1	B	141	LYS
2	C	20	ILE
2	D	20	ILE
2	C	53	PRO
2	D	145	ILE
2	D	53	PRO
2	C	13	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	421/460 (92%)	357 (85%)	64 (15%)	3	17
1	B	415/460 (90%)	357 (86%)	58 (14%)	3	19
2	C	120/128 (94%)	99 (82%)	21 (18%)	2	12
2	D	120/128 (94%)	99 (82%)	21 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1076/1176 (92%)	912 (85%)	164 (15%)	3 17

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	11	GLU
1	A	20	SER
1	A	31	MET
1	A	62	VAL
1	A	63	VAL
1	A	68	ILE
1	A	93	LEU
1	A	101	ILE
1	A	105	ASN
1	A	113	ILE
1	A	116	LEU
1	A	133	THR
1	A	142	LYS
1	A	149	THR
1	A	156	ASN
1	A	158	LEU
1	A	160	GLN
1	A	169	HIS
1	A	195	MET
1	A	197	ILE
1	A	216	LEU
1	A	222	SER
1	A	225	GLU
1	A	232	THR
1	A	234	ILE
1	A	239	LEU
1	A	243	ASN
1	A	250	VAL
1	A	257	ASN
1	A	263	LEU
1	A	264	LYS
1	A	270	GLN
1	A	276	VAL
1	A	280	GLU
1	A	297	HIS
1	A	310	ILE

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	315	ARG
1	A	316	THR
1	A	317	ASP
1	A	320	GLU
1	A	353	PHE
1	A	354	ASP
1	A	372	GLU
1	A	374	ILE
1	A	389	VAL
1	A	392	PHE
1	A	394	ILE
1	A	399	ILE
1	A	407	LYS
1	A	420	LYS
1	A	421	ASP
1	A	427	LEU
1	A	432	LYS
1	A	458	ASP
1	A	463	ILE
1	A	468	LEU
1	A	477	ASP
1	A	483	ILE
1	A	500	ILE
1	A	518	ILE
1	A	519	LEU
1	A	528	ARG
1	B	3	CYS
1	B	11	GLU
1	B	20	SER
1	B	27	ASN
1	B	31	MET
1	B	62	VAL
1	B	63	VAL
1	B	68	ILE
1	B	93	LEU
1	B	101	ILE
1	B	113	ILE
1	B	116	LEU
1	B	133	THR
1	B	142	LYS
1	B	149	THR

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Mol	Chain	Res	Type
1	B	156	ASN
1	B	158	LEU
1	B	160	GLN
1	B	195	MET
1	B	197	ILE
1	B	203	LEU
1	B	211	ASP
1	B	216	LEU
1	B	233	GLU
1	B	242	THR
1	B	261	GLU
1	B	276	VAL
1	B	282	CYS
1	B	284	ASP
1	B	289	ILE
1	B	292	LEU
1	B	302	TRP
1	B	305	LEU
1	B	307	GLU
1	B	308	THR
1	B	322	ASN
1	B	324	ILE
1	B	353	PHE
1	B	354	ASP
1	B	372	GLU
1	B	374	ILE
1	B	389	VAL
1	B	392	PHE
1	B	394	ILE
1	B	399	ILE
1	B	407	LYS
1	B	420	LYS
1	B	421	ASP
1	B	427	LEU
1	B	432	LYS
1	B	458	ASP
1	B	463	ILE
1	B	468	LEU
1	B	477	ASP
1	B	483	ILE
1	B	500	ILE
1	B	518	ILE

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Mol	Chain	Res	Type
1	B	519	LEU
2	C	27	PHE
2	C	29	ILE
2	C	30	LEU
2	C	38	LYS
2	C	47	GLN
2	C	60	MET
2	C	73	HIS
2	C	74	GLU
2	C	78	ILE
2	C	91	GLU
2	C	94	GLU
2	C	98	LYS
2	C	114	ILE
2	C	116	GLU
2	C	118	LYS
2	C	120	ARG
2	C	121	LEU
2	C	123	ARG
2	C	140	GLU
2	C	141	LYS
2	C	146	GLU
2	D	27	PHE
2	D	29	ILE
2	D	30	LEU
2	D	38	LYS
2	D	47	GLN
2	D	60	MET
2	D	73	HIS
2	D	74	GLU
2	D	78	ILE
2	D	91	GLU
2	D	94	GLU
2	D	98	LYS
2	D	114	ILE
2	D	116	GLU
2	D	118	LYS
2	D	120	ARG
2	D	121	LEU
2	D	123	ARG
2	D	140	GLU
2	D	141	LYS

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Mol	Chain	Res	Type
2	D	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	66	ASN
1	A	105	ASN
1	A	110	HIS
1	A	156	ASN
1	A	160	GLN
1	A	166	ASN
1	A	169	HIS
1	A	241	HIS
1	A	256	ASN
1	A	257	ASN
1	A	270	GLN
1	A	297	HIS
1	A	313	ASN
1	A	373	ASN
1	A	441	HIS
1	B	27	ASN
1	B	66	ASN
1	B	75	GLN
1	B	105	ASN
1	B	156	ASN
1	B	256	ASN
1	B	270	GLN
1	B	271	ASN
1	B	297	HIS
1	B	373	ASN
1	B	441	HIS
2	C	18	ASN
2	C	46	ASN
2	C	47	GLN
2	D	18	ASN
2	D	46	ASN
2	D	47	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TBR	B	2769	-	0,36,36	-	-	-		
3	TBR	A	4769	-	0,36,36	-	-	-		
3	TBR	B	8769	-	0,36,36	-	-	-		
3	TBR	A	6769	-	0,36,36	-	-	-		
3	TBR	B	3769	-	0,36,36	-	-	-		
3	TBR	B	7769	-	0,36,36	-	-	-		
3	TBR	A	5769	-	0,36,36	-	-	-		
3	TBR	A	1769	-	0,36,36	-	-	-		

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.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2769	TBR	1	0
3	A	6769	TBR	3	0
3	B	3769	TBR	2	0
3	B	7769	TBR	2	0
3	A	5769	TBR	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	495/540 (91%)	-0.07	12 (2%) 59 34	64, 102, 104, 115	2 (0%)
1	B	485/540 (89%)	-0.19	7 (1%) 73 46	86, 103, 120, 126	5 (1%)
2	C	138/150 (92%)	-0.09	2 (1%) 73 46	89, 105, 114, 116	1 (0%)
2	D	138/150 (92%)	-0.27	2 (1%) 73 46	88, 105, 114, 116	2 (1%)
All	All	1256/1380 (91%)	-0.14	23 (1%) 67 40	64, 103, 114, 126	10 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	LEU	4.4
1	A	160	GLN	3.4
1	B	504	PHE	3.1
1	A	75	GLN	3.0
1	B	271	ASN	3.0
1	B	107	CYS	3.0
1	A	103	GLY	2.8
2	C	119	GLU	2.8
2	D	87	CYS	2.8
1	B	159	ASP	2.8
1	B	293	GLY	2.6
1	A	18	VAL	2.6
1	A	8	GLY	2.5
1	A	499	GLU	2.4
1	A	429	ILE	2.4
1	A	73	PHE	2.4
1	A	411	MET	2.4
1	A	234	ILE	2.4
1	A	419	ALA	2.3
2	C	134	VAL	2.1
1	A	53	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	25	LEU	2.0
1	B	480	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TBR	B	7769	18/18	0.74	0.19	79,159,374,500	18
3	TBR	A	4769	18/18	0.81	0.10	151,222,500,500	18
3	TBR	B	2769	18/18	0.86	0.20	25,81,98,244	18
3	TBR	B	8769	18/18	0.86	0.22	51,146,180,230	18
3	TBR	B	3769	18/18	0.89	0.14	122,181,265,500	18
3	TBR	A	5769	18/18	0.90	0.10	72,127,269,500	18
3	TBR	A	6769	18/18	0.91	0.11	83,119,191,196	18
3	TBR	A	1769	18/18	0.97	0.07	67,105,143,170	18

6.5 Other polymers [i](#)

There are no such residues in this entry.