



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 PM UTC

PDB ID : 3E4B / pdb_00003e4b
Title : Crystal structure of AlgK from Pseudomonas fluorescens WCS374r
Authors : Keiski, C.-L.; Harwich, M.; Jain, S.; Neculai, A.M.; Yip, P.; Robinson, H.; Whitney, J.C.; Burrows, L.L.; Ohman, D.E.; Howell, P.L.
Deposited on : 2008-08-11
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

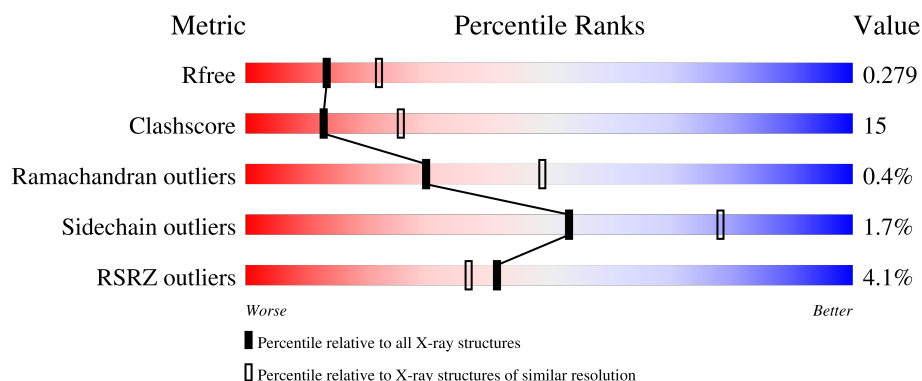
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	452	
1	B	452	
1	C	452	
1	D	452	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12341 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 AlgK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2988	1877	526	579	6			
1	B	405	Total	C	N	O	S	0	0	0
			3045	1915	530	594	6			
1	C	405	Total	C	N	O	S	0	0	0
			3057	1918	533	600	6			
1	D	316	Total	C	N	O	S	0	0	0
			2371	1493	407	466	5			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

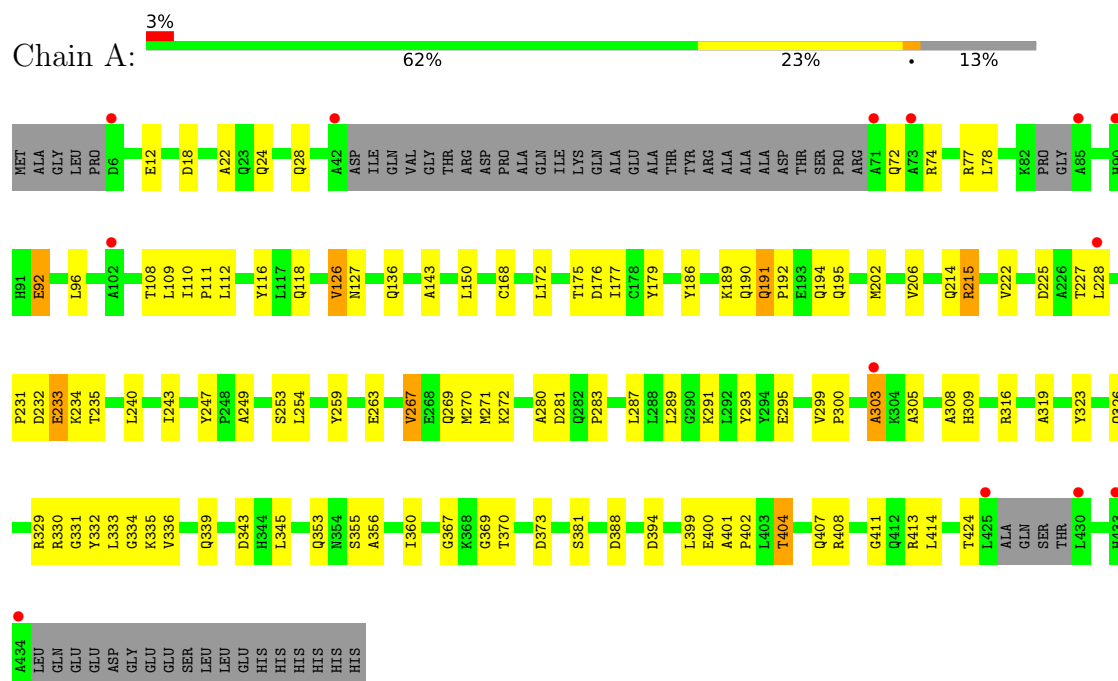
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	197	Total	O	0	0
			197	197		
4	B	222	Total	O	0	0
			222	222		
4	C	302	Total	O	0	0
			302	302		
4	D	132	Total	O	0	0
			132	132		

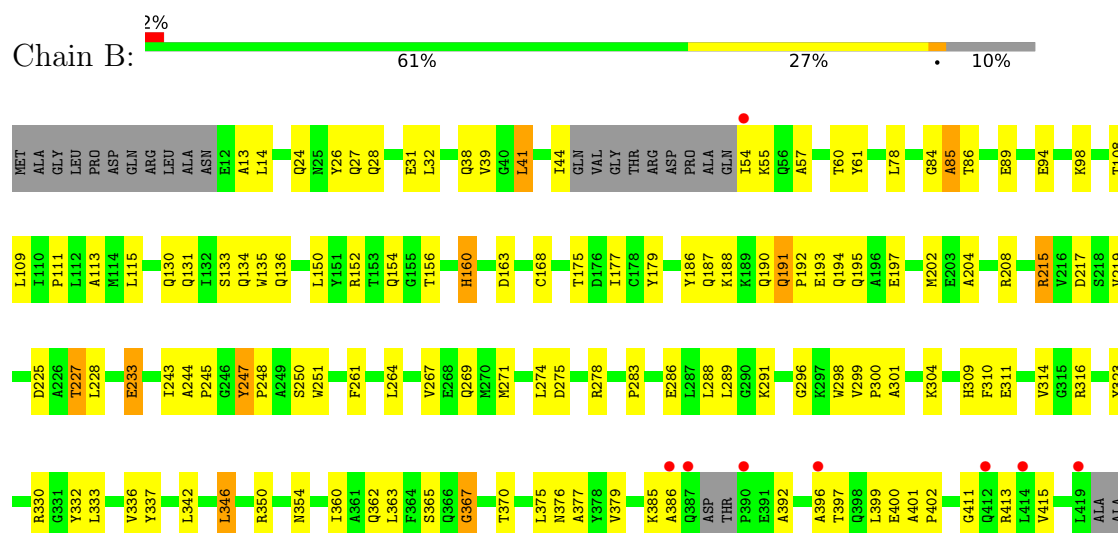
3 Residue-property plots

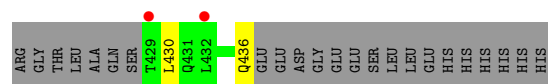
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: AlgK

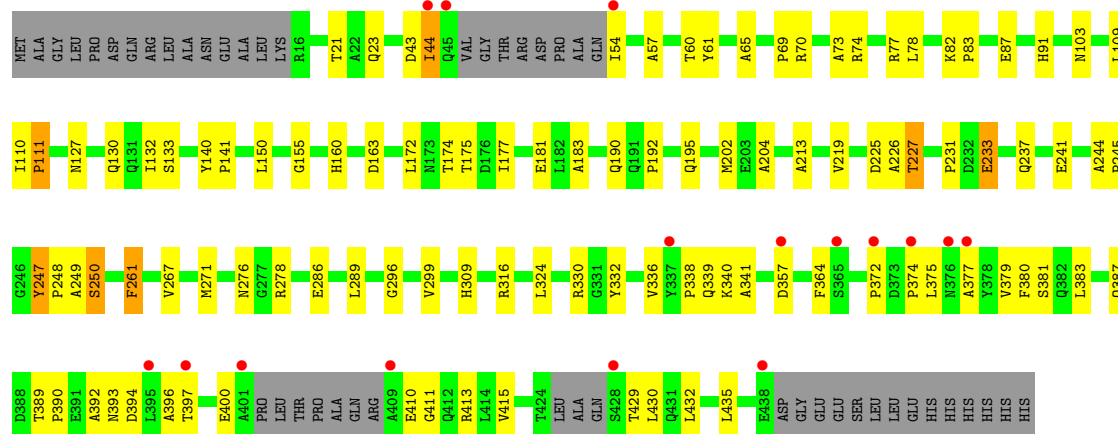


• Molecule 1: AlgK

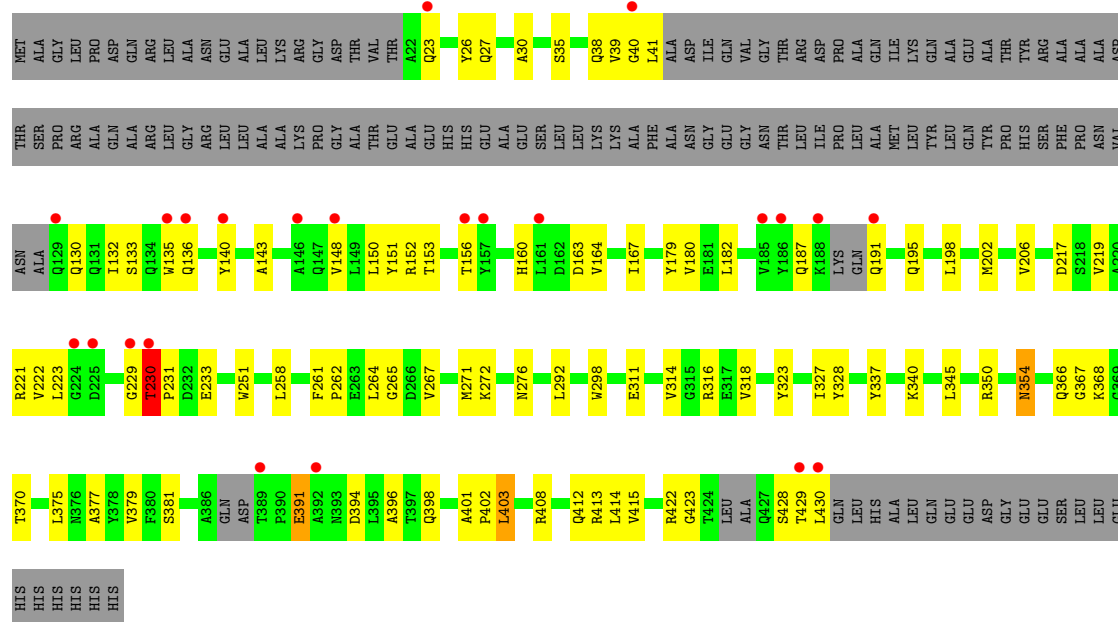




• Molecule 1: AlgK



• Molecule 1: AlgK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.09Å 107.82Å 119.03Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	49.05 – 2.50 49.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.05-2.50) 100.0 (49.05-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.280 0.220 , 0.279	Depositor DCC
R_{free} test set	3540 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12341	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: CL, GOL

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	0.59	0/3039	1.07	20/4129 (0.5%)
1	B	0.63	0/3100	1.05	22/4217 (0.5%)
1	C	0.69	0/3111	1.04	12/4230 (0.3%)
1	D	0.64	0/2411	1.08	16/3277 (0.5%)
All	All	0.64	0/11661	1.06	70/15853 (0.4%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	GLN	N-CA-C	-9.31	102.49	114.04
1	C	65	ALA	N-CA-C	8.77	121.63	111.11
1	B	247	TYR	CA-C-N	8.59	128.17	119.24
1	B	247	TYR	C-N-CA	8.59	128.17	119.24
1	B	13	ALA	N-CA-C	-8.57	102.58	113.72
1	A	191	GLN	CA-C-N	7.84	127.39	119.24
1	A	191	GLN	C-N-CA	7.84	127.39	119.24
1	C	247	TYR	CA-C-N	7.79	129.57	119.84
1	C	247	TYR	C-N-CA	7.79	129.57	119.84
1	A	263	GLU	N-CA-C	7.37	121.91	113.15
1	A	12	GLU	N-CA-C	-7.34	103.95	113.12
1	C	213	ALA	N-CA-C	-7.25	103.31	111.14
1	D	413	ARG	N-CA-C	-7.20	104.12	113.12
1	D	354	ASN	N-CA-C	7.02	121.29	112.87
1	A	303	ALA	N-CA-C	6.95	118.64	111.14
1	A	72	GLN	N-CA-C	-6.41	104.72	112.54
1	A	388	ASP	N-CA-C	6.28	118.25	110.91
1	A	126	VAL	N-CA-C	6.08	118.13	108.89
1	A	249	ALA	N-CA-C	-6.07	104.98	112.38
1	C	324	LEU	N-CA-C	-5.97	104.89	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	LYS	N-CA-C	-5.96	105.11	112.38
1	D	230	THR	CA-C-N	5.90	126.39	120.14
1	D	230	THR	C-N-CA	5.90	126.39	120.14
1	D	429	THR	N-CA-C	5.90	119.16	109.72
1	B	354	ASN	N-CA-C	5.88	118.47	111.71
1	A	18	ASP	N-CA-C	-5.82	105.02	111.36
1	D	251	TRP	N-CA-C	-5.80	105.04	111.36
1	C	204	ALA	N-CA-C	-5.76	104.90	111.07
1	B	430	LEU	N-CA-C	5.73	118.76	110.28
1	A	92	GLU	N-CA-C	-5.72	105.13	111.36
1	A	172	LEU	N-CA-C	5.71	118.23	111.33
1	B	298	TRP	N-CA-C	-5.71	105.04	112.23
1	B	136	GLN	N-CA-C	-5.67	105.00	111.07
1	D	191	GLN	CA-C-N	5.66	125.02	118.85
1	D	191	GLN	C-N-CA	5.66	125.02	118.85
1	B	191	GLN	CA-C-N	5.66	125.12	119.24
1	B	191	GLN	C-N-CA	5.66	125.12	119.24
1	B	275	ASP	N-CA-C	-5.64	105.21	111.36
1	A	373	ASP	CA-C-N	5.50	125.59	119.32
1	A	373	ASP	C-N-CA	5.50	125.59	119.32
1	C	261	PHE	CA-C-N	5.50	125.33	119.28
1	C	261	PHE	C-N-CA	5.50	125.33	119.28
1	A	400	GLU	N-CA-C	-5.45	106.79	113.50
1	A	179	TYR	N-CA-C	-5.43	105.52	111.82
1	C	276	ASN	N-CA-C	-5.42	105.27	111.07
1	A	168	CYS	N-CA-C	5.36	119.08	112.54
1	A	267	VAL	N-CA-C	-5.24	104.71	112.04
1	D	140	TYR	CA-C-N	5.24	124.42	118.97
1	D	140	TYR	C-N-CA	5.24	124.42	118.97
1	B	413	ARG	N-CA-C	-5.23	106.41	112.89
1	B	243	ILE	N-CA-C	5.22	120.23	113.07
1	D	337	TYR	CA-C-N	5.21	124.66	119.24
1	D	337	TYR	C-N-CA	5.21	124.66	119.24
1	D	414	LEU	N-CA-C	-5.17	105.65	111.28
1	C	289	LEU	N-CA-C	-5.14	105.75	111.36
1	C	374	PRO	N-CA-C	5.13	120.28	113.40
1	B	215	ARG	CG-CD-NE	-5.13	100.72	112.00
1	A	404	THR	N-CA-C	-5.12	102.59	110.07
1	B	187	GLN	N-CA-C	-5.12	105.39	111.69
1	D	428	SER	N-CA-C	-5.11	101.94	110.17
1	B	204	ALA	N-CA-C	-5.11	105.61	111.07
1	D	403	LEU	N-CA-C	5.10	117.82	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	SER	N-CA-C	-5.08	105.82	111.36
1	B	61	TYR	N-CA-C	-5.06	105.84	111.36
1	C	372	PRO	N-CA-C	5.06	122.89	112.47
1	B	160	HIS	N-CA-C	5.05	118.53	111.56
1	B	168	CYS	N-CA-C	5.04	117.67	111.82
1	B	251	TRP	N-CA-C	-5.04	105.88	112.23
1	B	269	GLN	N-CA-C	-5.04	105.79	111.28
1	A	231	PRO	N-CA-C	5.00	119.04	111.19

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	2988	0	2888	85	0
1	B	3045	0	2896	91	0
1	C	3057	0	2913	99	0
1	D	2371	0	2243	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	8	0	0
4	A	197	0	0	7	0
4	B	222	0	0	8	0
4	C	302	0	0	6	0
4	D	132	0	0	3	0
All	All	12341	0	10972	340	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 15.

All (340) 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:B:202:MET:HE1	1:B:219:VAL:HG21	1.19	1.18
1:C:202:MET:HE1	1:C:219:VAL:HG21	1.34	1.09
1:B:202:MET:HE1	1:B:219:VAL:CG2	1.94	0.98
1:B:202:MET:CE	1:B:219:VAL:HG21	2.02	0.90
1:C:387:GLN:HG2	1:C:389:THR:HG23	1.52	0.90
1:A:191:GLN:HB3	1:A:194:GLN:OE1	1.72	0.89
1:C:330:ARG:HH11	1:C:330:ARG:HB3	1.39	0.85
1:D:391:GLU:H	1:D:391:GLU:CD	1.84	0.85
1:C:202:MET:HE1	1:C:219:VAL:CG2	2.06	0.85
1:C:233:GLU:HG2	1:C:261:PHE:CD1	2.13	0.84
1:A:303:ALA:HB1	1:A:333:LEU:HD23	1.59	0.83
1:B:191:GLN:HB3	1:B:194:GLN:OE1	1.76	0.83
1:C:336:VAL:O	1:C:338:PRO:HD3	1.78	0.83
1:C:60:THR:HG23	1:C:61:TYR:H	1.43	0.83
1:B:60:THR:HB	4:B:716:HOH:O	1.77	0.83
1:B:274:LEU:O	1:B:278:ARG:HG3	1.78	0.82
1:C:202:MET:CE	1:C:219:VAL:HG21	2.10	0.81
1:D:148:VAL:HG22	1:D:164:VAL:HG22	1.63	0.79
1:B:233:GLU:HG2	1:B:261:PHE:CD1	2.20	0.77
1:B:367:GLY:HA2	1:B:370:THR:O	1.83	0.77
1:C:74:ARG:NH1	1:C:74:ARG:HB2	2.00	0.77
1:C:54:ILE:HG12	1:C:54:ILE:O	1.84	0.76
1:C:430:LEU:HB3	1:C:432:LEU:HD11	1.66	0.76
1:C:390:PRO:O	1:C:394:ASP:HB2	1.87	0.75
1:A:369:GLY:C	1:B:436:GLN:HG3	2.11	0.74
1:A:214:GLN:O	1:A:214:GLN:HG2	1.88	0.73
1:C:226:ALA:HA	1:C:231:PRO:HG3	1.71	0.73
1:D:233:GLU:HB2	1:D:264:LEU:CD2	2.19	0.72
1:B:175:THR:HG22	1:B:177:ILE:HG22	1.72	0.72
1:B:26:TYR:CE1	1:B:41:LEU:HD11	2.25	0.71
1:B:57:ALA:O	1:B:60:THR:HG22	1.90	0.71
1:A:335:LYS:HG2	1:A:336:VAL:H	1.54	0.71
1:B:311:GLU:O	1:B:314:VAL:HG22	1.91	0.71
1:B:278:ARG:HH11	1:B:278:ARG:HB3	1.54	0.71
1:B:225:ASP:OD1	1:B:227:THR:HB	1.91	0.70
1:A:331:GLY:HA3	1:A:336:VAL:HG22	1.71	0.70
1:B:26:TYR:CZ	1:B:41:LEU:HD11	2.27	0.69
1:C:339:GLN:HG3	1:C:340:LYS:H	1.56	0.69
1:D:233:GLU:HB2	1:D:264:LEU:HD23	1.73	0.69
1:A:22:ALA:HA	1:A:118:GLN:HE21	1.58	0.69
1:B:385:LYS:HA	1:B:392:ALA:HB1	1.74	0.68
1:D:272:LYS:HE2	1:D:276:ASN:HD21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ALA:HA	1:C:195:GLN:HE22	1.58	0.67
1:B:44:ILE:CG2	1:B:78:LEU:HD13	2.24	0.67
1:B:186:TYR:HB3	1:B:195:GLN:HG2	1.74	0.67
1:C:432:LEU:N	1:C:432:LEU:HD12	2.10	0.67
1:B:109:LEU:HD21	1:B:135:TRP:CE3	2.29	0.67
1:A:353:GLN:HE21	1:A:355:SER:HB2	1.59	0.66
1:A:299:VAL:HB	1:A:300:PRO:HD2	1.78	0.66
1:A:330:ARG:HD2	1:A:332:TYR:CZ	2.30	0.66
1:B:286:GLU:OE1	1:B:309:HIS:HD2	1.80	0.65
1:A:411:GLY:HA2	1:A:414:LEU:HD12	1.77	0.65
1:B:233:GLU:HG2	1:B:261:PHE:CG	2.31	0.65
1:C:87:GLU:HG2	1:C:91:HIS:CE1	2.32	0.65
1:A:413:ARG:HG2	1:A:413:ARG:HH11	1.62	0.64
1:B:160:HIS:HD2	1:B:163:ASP:OD2	1.80	0.64
1:B:108:THR:C	1:B:111:PRO:HD2	2.21	0.64
1:D:318:VAL:HG23	4:D:704:HOH:O	1.98	0.64
1:C:57:ALA:HA	1:C:60:THR:HG22	1.79	0.64
1:C:375:LEU:O	1:C:379:VAL:HG23	1.98	0.64
1:C:60:THR:HG23	1:C:61:TYR:N	2.12	0.64
1:D:264:LEU:O	1:D:264:LEU:HD12	1.98	0.63
1:A:92:GLU:O	1:A:96:LEU:HG	1.99	0.63
1:B:190:GLN:O	1:B:192:PRO:HD3	1.99	0.63
1:C:411:GLY:O	1:C:415:VAL:HG23	1.98	0.63
1:C:364:PHE:HB2	1:C:377:ALA:HB2	1.81	0.62
1:C:233:GLU:HG2	1:C:261:PHE:CG	2.34	0.62
1:C:330:ARG:HB3	1:C:330:ARG:NH1	2.10	0.62
1:A:240:LEU:HB2	1:A:254:LEU:HD21	1.80	0.62
1:D:156:THR:HB	1:D:160:HIS:HE1	1.64	0.62
1:C:247:TYR:O	1:C:250:SER:HB2	1.99	0.61
1:D:40:GLY:O	1:D:41:LEU:CB	2.48	0.61
1:C:57:ALA:O	1:C:60:THR:HG22	2.00	0.61
1:A:225:ASP:OD1	1:A:227:THR:HB	2.01	0.61
1:A:291:LYS:O	1:A:295:GLU:HG2	2.01	0.60
1:C:339:GLN:CG	1:C:340:LYS:H	2.14	0.60
1:B:291:LYS:HE3	1:B:323:TYR:OH	2.02	0.60
1:D:202:MET:CE	1:D:219:VAL:HG21	2.31	0.60
1:C:225:ASP:OD1	1:C:227:THR:HB	2.02	0.60
1:B:208:ARG:HG2	1:B:208:ARG:HH11	1.67	0.59
1:B:32:LEU:HD21	1:B:152:ARG:CZ	2.32	0.59
1:A:335:LYS:HG2	1:A:336:VAL:N	2.18	0.59
1:C:387:GLN:HG2	1:C:389:THR:CG2	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD23	1:A:289:LEU:C	2.29	0.58
1:B:283:PRO:HD2	4:B:598:HOH:O	2.04	0.58
1:C:127:ASN:HB3	1:C:130:GLN:HB2	1.86	0.58
1:A:269:GLN:O	1:A:272:LYS:N	2.35	0.57
1:B:278:ARG:HB3	1:B:278:ARG:NH1	2.19	0.57
1:A:28:GLN:HB3	4:A:524:HOH:O	2.04	0.57
1:C:190:GLN:O	1:C:192:PRO:HD3	2.05	0.57
1:D:156:THR:HB	1:D:160:HIS:CE1	2.39	0.57
1:A:291:LYS:HE3	1:A:323:TYR:OH	2.04	0.57
1:B:299:VAL:HG22	1:B:300:PRO:HD2	1.87	0.57
1:B:57:ALA:O	1:B:60:THR:CG2	2.52	0.57
1:B:289:LEU:HD23	1:B:309:HIS:CD2	2.40	0.57
1:A:186:TYR:CB	1:A:195:GLN:HG2	2.35	0.56
1:A:186:TYR:HB3	1:A:195:GLN:HG2	1.87	0.56
1:D:187:GLN:NE2	1:D:230:THR:O	2.39	0.56
1:D:153:THR:HG22	4:D:763:HOH:O	2.06	0.56
1:C:233:GLU:HG2	1:C:261:PHE:CE1	2.40	0.56
1:A:394:ASP:HB3	4:A:585:HOH:O	2.06	0.56
1:B:330:ARG:CZ	1:B:332:TYR:OH	2.54	0.55
1:C:109:LEU:C	1:C:109:LEU:HD23	2.31	0.55
1:C:330:ARG:NH1	1:C:332:TYR:CE1	2.75	0.55
1:D:35:SER:HG	1:D:38:GLN:CD	2.15	0.55
1:A:78:LEU:HD23	1:A:78:LEU:C	2.31	0.55
1:A:136:GLN:HG3	1:A:143:ALA:HB1	1.89	0.55
1:D:202:MET:HE1	1:D:219:VAL:CB	2.36	0.55
1:D:202:MET:O	1:D:206:VAL:HG23	2.07	0.55
1:B:377:ALA:HB1	1:B:399:LEU:HD13	1.88	0.55
1:C:155:GLY:HA2	4:C:609:HOH:O	2.06	0.55
1:B:296:GLY:HA2	1:B:299:VAL:O	2.07	0.55
1:C:110:ILE:HB	1:C:111:PRO:HD3	1.88	0.54
1:A:289:LEU:HD22	1:A:309:HIS:ND1	2.22	0.54
1:C:57:ALA:CA	1:C:60:THR:HG22	2.37	0.54
1:B:39:VAL:HG23	1:B:41:LEU:HD13	1.88	0.54
1:A:283:PRO:HG3	1:A:316:ARG:CZ	2.37	0.54
1:A:150:LEU:C	1:A:150:LEU:HD23	2.33	0.54
1:C:57:ALA:O	1:C:60:THR:CG2	2.55	0.54
1:C:74:ARG:HB2	1:C:74:ARG:HH11	1.71	0.54
1:B:14:LEU:HD12	1:B:14:LEU:H	1.73	0.54
1:B:131:GLN:O	1:B:134:GLN:HB3	2.08	0.54
1:A:281:ASP:O	1:A:283:PRO:HD3	2.07	0.54
1:C:174:THR:HG23	4:C:720:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:LEU:O	1:D:379:VAL:HG23	2.08	0.54
1:B:188:LYS:NZ	4:B:652:HOH:O	2.36	0.53
1:A:331:GLY:CA	1:A:336:VAL:HG22	2.36	0.53
1:B:154:GLN:O	1:B:156:THR:HG23	2.07	0.53
1:A:289:LEU:HD23	1:A:289:LEU:O	2.09	0.53
1:C:78:LEU:HD23	1:C:78:LEU:C	2.33	0.53
1:D:182:LEU:HB3	1:D:198:LEU:HD22	1.91	0.53
1:C:73:ALA:HB1	1:C:77:ARG:HH12	1.74	0.53
1:B:375:LEU:O	1:B:379:VAL:HG23	2.09	0.53
1:A:326:GLN:OE1	1:A:326:GLN:HA	2.07	0.53
1:D:316:ARG:HH11	1:D:316:ARG:HG3	1.73	0.53
1:A:280:ALA:O	1:A:281:ASP:HB3	2.07	0.53
1:B:360:ILE:O	1:B:363:LEU:HB3	2.09	0.53
1:A:408:ARG:HD3	4:A:560:HOH:O	2.09	0.52
1:A:269:GLN:OE1	1:A:269:GLN:HA	2.08	0.52
1:B:247:TYR:O	1:B:250:SER:HB2	2.09	0.52
1:A:175:THR:HG22	1:A:177:ILE:HG22	1.90	0.52
1:A:190:GLN:C	1:A:192:PRO:HD3	2.35	0.52
1:B:44:ILE:HG22	1:B:44:ILE:O	2.09	0.52
1:C:109:LEU:HD23	1:C:109:LEU:O	2.09	0.52
1:A:190:GLN:O	1:A:192:PRO:HD3	2.09	0.52
1:C:57:ALA:C	1:C:60:THR:HG22	2.35	0.52
1:C:286:GLU:OE1	1:C:309:HIS:HD2	1.92	0.52
1:D:163:ASP:O	1:D:167:ILE:HG13	2.09	0.52
1:C:74:ARG:HH11	1:C:74:ARG:CB	2.23	0.52
1:B:86:THR:OG1	1:B:89:GLU:HG3	2.10	0.52
1:B:190:GLN:C	1:B:192:PRO:HD3	2.35	0.52
1:A:24:GLN:O	1:A:28:GLN:HG3	2.10	0.51
1:A:243:ILE:HB	4:A:646:HOH:O	2.10	0.51
1:A:289:LEU:HD21	1:A:293:TYR:CE2	2.45	0.51
1:A:332:TYR:C	1:A:334:GLY:H	2.19	0.51
1:A:77:ARG:NH2	4:A:599:HOH:O	2.43	0.51
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.91	0.51
1:B:94:GLU:O	1:B:98:LYS:HG3	2.09	0.51
1:C:336:VAL:C	1:C:338:PRO:HD3	2.35	0.51
1:A:202:MET:O	1:A:206:VAL:HG23	2.11	0.51
1:D:233:GLU:HB2	1:D:264:LEU:HD21	1.91	0.51
1:B:44:ILE:HG22	1:B:78:LEU:HD13	1.92	0.51
1:D:367:GLY:HA2	1:D:370:THR:O	2.11	0.51
1:A:259:TYR:HE2	1:A:295:GLU:OE2	1.94	0.51
1:B:310:PHE:CE2	1:B:323:TYR:HB3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:O	1:C:133:SER:OG	2.22	0.50
1:D:132:ILE:HA	1:D:135:TRP:CE3	2.47	0.50
1:A:413:ARG:HG2	1:A:413:ARG:NH1	2.27	0.50
1:A:109:LEU:HD23	1:A:109:LEU:C	2.37	0.50
1:C:316:ARG:HG3	1:C:316:ARG:HH11	1.77	0.50
1:C:330:ARG:NH1	1:C:332:TYR:HE1	2.10	0.49
1:B:401:ALA:HB3	1:B:402:PRO:HD3	1.95	0.49
1:C:396:ALA:O	1:C:400:GLU:HG3	2.13	0.49
1:B:208:ARG:HG2	1:B:208:ARG:NH1	2.26	0.49
1:C:430:LEU:HB3	1:C:432:LEU:CD1	2.40	0.49
1:C:430:LEU:CB	1:C:432:LEU:HD11	2.41	0.49
1:D:202:MET:HE1	1:D:219:VAL:HG11	1.95	0.49
1:C:175:THR:HG22	1:C:177:ILE:HG22	1.95	0.49
1:B:38:GLN:NE2	1:B:177:ILE:HB	2.27	0.48
1:C:60:THR:CG2	1:C:61:TYR:H	2.20	0.48
1:D:272:LYS:HE2	1:D:276:ASN:ND2	2.26	0.48
1:B:197:GLU:OE1	1:B:197:GLU:HA	2.14	0.48
1:A:401:ALA:HB3	1:A:402:PRO:HD3	1.95	0.48
1:D:258:LEU:HD11	1:D:265:GLY:HA3	1.95	0.48
1:B:24:GLN:O	1:B:28:GLN:HG3	2.13	0.48
1:B:396:ALA:O	1:B:400:GLU:HB2	2.14	0.48
1:D:39:VAL:HG23	1:D:40:GLY:N	2.28	0.48
1:D:354:ASN:OD1	1:D:354:ASN:N	2.47	0.48
1:D:366:GLN:O	1:D:368:LYS:HG2	2.13	0.48
1:D:403:LEU:O	1:D:408:ARG:NH2	2.38	0.48
1:A:108:THR:C	1:A:111:PRO:HD2	2.38	0.48
1:C:57:ALA:HA	1:C:60:THR:CG2	2.44	0.48
1:C:202:MET:HE1	1:C:219:VAL:CB	2.42	0.48
1:D:30:ALA:HB2	4:D:699:HOH:O	2.14	0.48
1:B:130:GLN:HG3	4:B:660:HOH:O	2.14	0.48
1:B:217:ASP:OD2	1:B:250:SER:OG	2.30	0.47
1:B:283:PRO:HG3	1:B:316:ARG:CZ	2.44	0.47
1:B:411:GLY:O	1:B:415:VAL:HG23	2.14	0.47
1:D:292:LEU:HD22	1:D:298:TRP:HB2	1.96	0.47
1:B:27:GLN:O	1:B:31:GLU:HG2	2.14	0.47
1:D:179:TYR:CD1	1:D:198:LEU:HD11	2.49	0.47
1:B:278:ARG:HD2	1:B:286:GLU:OE2	2.14	0.47
1:C:397:THR:O	1:C:400:GLU:HB2	2.15	0.47
1:A:74:ARG:HB3	4:A:540:HOH:O	2.15	0.47
1:A:305:ALA:O	1:A:308:ALA:HB3	2.14	0.47
1:B:436:GLN:HB2	4:B:773:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:VAL:HG13	1:D:222:VAL:HG21	1.96	0.47
1:D:258:LEU:CD1	1:D:265:GLY:HA3	2.45	0.47
1:D:412:GLN:O	1:D:412:GLN:HG3	2.14	0.47
1:D:377:ALA:O	1:D:381:SER:HB2	2.15	0.47
1:A:367:GLY:HA2	1:A:370:THR:O	2.15	0.46
1:C:339:GLN:HG3	1:C:340:LYS:N	2.27	0.46
1:C:375:LEU:HD11	1:C:411:GLY:HA3	1.97	0.46
1:A:269:GLN:O	1:A:270:MET:C	2.58	0.46
1:D:261:PHE:O	1:D:262:PRO:C	2.58	0.46
1:C:316:ARG:HG3	1:C:316:ARG:NH1	2.31	0.46
1:C:339:GLN:CG	1:C:340:LYS:N	2.78	0.46
1:D:150:LEU:C	1:D:152:ARG:N	2.73	0.46
1:B:202:MET:HE1	1:B:219:VAL:CB	2.46	0.46
1:C:23:GLN:NE2	4:C:568:HOH:O	2.48	0.46
1:C:61:TYR:CE1	1:C:74:ARG:HD2	2.51	0.46
1:A:176:ASP:OD1	1:A:215:ARG:NE	2.48	0.46
1:D:264:LEU:O	1:D:264:LEU:CD1	2.63	0.46
1:A:326:GLN:HE22	1:A:329:ARG:HH21	1.64	0.46
1:A:243:ILE:CG2	1:A:247:TYR:HB3	2.46	0.46
1:A:287:LEU:HD21	1:A:319:ALA:HB3	1.98	0.46
1:C:267:VAL:O	1:C:271:MET:HG2	2.15	0.46
1:B:150:LEU:HD23	1:B:150:LEU:C	2.40	0.45
1:C:330:ARG:HH11	1:C:330:ARG:CB	2.20	0.45
1:D:202:MET:HE1	1:D:219:VAL:HG21	1.97	0.45
1:B:336:VAL:HG12	1:B:337:TYR:N	2.31	0.45
1:C:377:ALA:O	1:C:381:SER:HB2	2.17	0.45
1:D:391:GLU:CD	1:D:391:GLU:N	2.64	0.45
1:B:188:LYS:HE2	1:B:228:LEU:HD22	1.98	0.45
1:C:172:LEU:HD12	1:C:172:LEU:O	2.17	0.45
1:D:401:ALA:HB3	1:D:402:PRO:HD3	1.99	0.45
1:A:233:GLU:HG2	1:A:234:LYS:H	1.81	0.45
1:C:160:HIS:HD2	1:C:163:ASP:OD2	2.00	0.45
1:C:233:GLU:H	1:C:233:GLU:CD	2.24	0.45
1:A:232:ASP:OD1	1:A:235:THR:OG1	2.32	0.45
1:B:193:GLU:HG3	4:B:710:HOH:O	2.17	0.45
1:D:150:LEU:C	1:D:152:ARG:H	2.25	0.45
1:D:160:HIS:HB3	1:D:163:ASP:HB2	1.99	0.45
1:D:202:MET:HE2	1:D:219:VAL:HG21	1.98	0.45
1:C:21:THR:HG22	4:C:624:HOH:O	2.17	0.44
1:C:140:TYR:HA	1:C:141:PRO:HD2	1.85	0.44
1:A:175:THR:HA	4:A:526:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:NH1	1:B:278:ARG:CB	2.80	0.44
1:D:26:TYR:HB2	1:D:27:GLN:NE2	2.32	0.44
1:D:398:GLN:O	1:D:402:PRO:HD3	2.17	0.44
1:A:326:GLN:NE2	1:A:329:ARG:HH21	2.15	0.44
1:C:70:ARG:HG3	1:C:70:ARG:HH11	1.83	0.44
1:C:410:GLU:O	1:C:413:ARG:HB3	2.17	0.44
1:B:113:ALA:HB2	1:B:135:TRP:HZ3	1.82	0.44
1:B:342:LEU:O	1:B:346:LEU:HB2	2.18	0.44
1:C:429:THR:HG22	1:D:350:ARG:NH2	2.33	0.44
1:D:323:TYR:O	1:D:327:ILE:HG13	2.18	0.44
1:D:328:TYR:CD2	1:D:340:LYS:HB3	2.52	0.44
1:A:22:ALA:HA	1:A:118:GLN:NE2	2.31	0.44
1:C:160:HIS:HE1	4:C:696:HOH:O	1.99	0.44
1:C:380:PHE:HA	1:C:383:LEU:HB2	2.00	0.44
1:B:304:LYS:HB2	1:C:130:GLN:NE2	2.33	0.44
1:C:73:ALA:HB1	1:C:77:ARG:NH1	2.33	0.44
1:C:78:LEU:HD23	1:C:78:LEU:O	2.18	0.44
1:A:381:SER:HB3	1:A:399:LEU:HD12	2.00	0.44
1:C:177:ILE:HG13	1:C:177:ILE:O	2.18	0.43
1:D:202:MET:HE1	1:D:219:VAL:HB	2.00	0.43
1:D:311:GLU:HA	1:D:314:VAL:HG23	2.00	0.43
1:A:356:ALA:O	1:A:360:ILE:HG13	2.19	0.43
1:B:108:THR:O	1:B:111:PRO:HD2	2.18	0.43
1:C:244:ALA:N	1:C:245:PRO:CD	2.81	0.43
1:C:340:LYS:O	1:C:341:ALA:C	2.61	0.43
1:A:233:GLU:HG2	1:A:234:LYS:N	2.33	0.43
1:A:404:THR:HG23	1:A:407:GLN:OE1	2.18	0.43
1:C:357:ASP:HB2	4:C:764:HOH:O	2.18	0.43
1:A:189:LYS:HB3	1:A:191:GLN:HG3	1.99	0.43
1:B:177:ILE:HG13	1:B:177:ILE:O	2.18	0.43
1:B:278:ARG:HD3	1:B:289:LEU:CD2	2.49	0.43
1:D:381:SER:OG	1:D:396:ALA:HA	2.19	0.43
1:A:267:VAL:O	1:A:271:MET:HG2	2.18	0.43
1:A:353:GLN:NE2	1:A:355:SER:HB2	2.27	0.43
1:D:23:GLN:O	1:D:27:GLN:HG2	2.19	0.43
1:D:379:VAL:HG13	1:D:415:VAL:CG2	2.48	0.43
1:A:331:GLY:HA2	1:A:335:LYS:O	2.19	0.43
1:C:278:ARG:HH11	1:C:278:ARG:HG2	1.83	0.43
1:B:278:ARG:HD3	1:B:289:LEU:HD22	2.00	0.43
1:C:60:THR:CG2	1:C:61:TYR:N	2.81	0.43
1:A:424:THR:O	1:A:424:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HA	4:B:606:HOH:O	2.17	0.42
1:A:110:ILE:N	1:A:111:PRO:CD	2.82	0.42
1:C:69:PRO:HG2	1:C:103:ASN:ND2	2.34	0.42
1:C:82:LYS:HA	1:C:83:PRO:HD3	1.90	0.42
1:A:222:VAL:O	1:A:228:LEU:HD12	2.20	0.42
1:C:248:PRO:C	1:C:250:SER:N	2.74	0.42
1:D:195:GLN:OE1	1:D:195:GLN:HA	2.20	0.42
1:D:422:ARG:O	1:D:423:GLY:C	2.63	0.42
1:A:126:VAL:HG12	1:A:127:ASN:N	2.35	0.42
1:B:54:ILE:HD13	1:B:54:ILE:HA	1.88	0.42
1:B:346:LEU:HD22	1:B:350:ARG:CZ	2.50	0.42
1:C:43:ASP:O	1:C:44:ILE:HG23	2.20	0.42
1:D:136:GLN:HB3	1:D:143:ALA:HB1	2.01	0.42
1:A:112:LEU:HD11	1:A:116:TYR:CZ	2.55	0.41
1:A:331:GLY:HA3	1:A:336:VAL:CG2	2.43	0.41
1:C:237:GLN:O	1:C:241:GLU:HG3	2.21	0.41
1:D:229:GLY:O	1:D:230:THR:C	2.63	0.41
1:B:244:ALA:N	1:B:245:PRO:CD	2.83	0.41
1:B:397:THR:HA	1:B:400:GLU:HB3	2.01	0.41
1:D:187:GLN:OE1	1:D:223:LEU:HD22	2.20	0.41
1:A:345:LEU:O	1:A:356:ALA:HB1	2.21	0.41
1:B:392:ALA:O	1:B:396:ALA:HB2	2.20	0.41
1:D:345:LEU:HD23	1:D:345:LEU:HA	1.91	0.41
1:C:296:GLY:HA2	1:C:299:VAL:O	2.20	0.41
1:D:267:VAL:O	1:D:271:MET:HG2	2.21	0.41
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.36	0.41
1:B:225:ASP:CG	4:B:682:HOH:O	2.63	0.41
1:B:376:ASN:HA	1:B:379:VAL:HG23	2.02	0.41
1:C:286:GLU:OE1	1:C:309:HIS:CD2	2.73	0.41
1:C:339:GLN:HA	1:D:430:LEU:CB	2.51	0.41
1:A:259:TYR:CE2	1:A:295:GLU:OE2	2.72	0.41
1:A:281:ASP:O	1:A:281:ASP:CG	2.63	0.41
1:A:339:GLN:O	1:A:343:ASP:HB2	2.21	0.41
1:B:267:VAL:O	1:B:271:MET:HG2	2.21	0.41
1:C:181:GLU:OE1	1:C:181:GLU:HA	2.21	0.41
1:C:377:ALA:O	1:C:381:SER:CB	2.68	0.41
1:D:133:SER:HA	1:D:136:GLN:HG2	2.02	0.41
1:A:186:TYR:HB2	1:A:195:GLN:HG2	2.02	0.41
1:A:289:LEU:HD22	1:A:309:HIS:CE1	2.56	0.41
1:B:362:GLN:HA	1:B:365:SER:OG	2.21	0.41
1:C:132:ILE:HD12	1:C:150:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:SER:HG	1:D:38:GLN:CG	2.33	0.40
1:D:230:THR:HA	1:D:231:PRO:HD2	1.89	0.40
1:B:248:PRO:C	1:B:250:SER:N	2.77	0.40
1:A:289:LEU:C	1:A:289:LEU:CD2	2.94	0.40
1:B:179:TYR:HB3	1:B:202:MET:HE3	2.03	0.40
1:C:392:ALA:O	1:C:393:ASN:C	2.65	0.40
1:D:150:LEU:O	1:D:152:ARG:N	2.54	0.40
1:D:217:ASP:O	1:D:221:ARG:HG3	2.21	0.40
1:B:84:GLY:O	1:B:85:ALA:C	2.64	0.40
1:B:333:LEU:HD23	1:B:333:LEU:HA	1.87	0.40
1:C:74:ARG:HB2	1:C:74:ARG:CZ	2.51	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	387/452 (86%)	367 (95%)	20 (5%)	0	100	100
1	B	397/452 (88%)	380 (96%)	14 (4%)	3 (1%)	16	31
1	C	397/452 (88%)	372 (94%)	24 (6%)	1 (0%)	36	55
1	D	306/452 (68%)	287 (94%)	17 (6%)	2 (1%)	18	34
All	All	1487/1808 (82%)	1406 (95%)	75 (5%)	6 (0%)	30	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ALA
1	B	386	ALA
1	C	249	ALA
1	D	151	TYR

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Mol	Chain	Res	Type
1	B	367	GLY
1	D	230	THR

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	287/351 (82%)	284 (99%)	3 (1%)	68	86
1	B	287/351 (82%)	280 (98%)	7 (2%)	43	70
1	C	292/351 (83%)	286 (98%)	6 (2%)	47	74
1	D	223/351 (64%)	221 (99%)	2 (1%)	70	87
All	All	1089/1404 (78%)	1071 (98%)	18 (2%)	53	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	233	GLU
1	A	253	SER
1	B	41	LEU
1	B	215	ARG
1	B	227	THR
1	B	233	GLU
1	B	264	LEU
1	B	288	LEU
1	B	346	LEU
1	C	44	ILE
1	C	111	PRO
1	C	227	THR
1	C	233	GLU
1	C	250	SER
1	C	435	LEU
1	D	391	GLU
1	D	394	ASP

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	90	HIS
1	A	118	GLN
1	A	129	GLN
1	A	136	GLN
1	A	147	GLN
1	A	154	GLN
1	A	214	GLN
1	A	309	HIS
1	A	351	ASN
1	A	353	GLN
1	A	362	GLN
1	A	366	GLN
1	A	387	GLN
1	B	160	HIS
1	B	201	GLN
1	B	309	HIS
1	B	339	GLN
1	B	417	GLN
1	C	23	GLN
1	C	24	GLN
1	C	72	GLN
1	C	125	ASN
1	C	130	GLN
1	C	131	GLN
1	C	160	HIS
1	C	187	GLN
1	C	190	GLN
1	C	191	GLN
1	C	195	GLN
1	C	309	HIS
1	C	362	GLN
1	C	433	HIS
1	D	214	GLN
1	D	269	GLN
1	D	351	ASN
1	D	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	C	455	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	D	453	-	5,5,5	0.13	0	5,5,5	0.33	0
3	GOL	C	453	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GOL	B	453	-	5,5,5	0.33	0	5,5,5	0.31	0

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	GOL	C	455	-	-	0/4/4/4	-
3	GOL	D	453	-	-	0/4/4/4	-
3	GOL	C	453	-	-	0/4/4/4	-
3	GOL	B	453	-	-	0/4/4/4	-

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/452 (87%)	0.22	13 (3%) 49 45	28, 50, 73, 83	0
1	B	405/452 (89%)	0.05	10 (2%) 58 54	23, 44, 90, 99	0
1	C	405/452 (89%)	0.03	16 (3%) 42 38	17, 38, 80, 94	0
1	D	316/452 (69%)	0.41	23 (7%) 21 19	26, 52, 84, 95	0
All	All	1521/1808 (84%)	0.17	62 (4%) 41 37	17, 46, 81, 99	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	LEU	4.6
1	C	401	ALA	4.5
1	A	71	ALA	4.4
1	D	188	LYS	4.3
1	B	390	PRO	4.0
1	D	161	LEU	3.9
1	C	357	ASP	3.9
1	A	430	LEU	3.8
1	B	387	GLN	3.5
1	A	434	ALA	3.5
1	D	135	TRP	3.4
1	C	409	ALA	3.3
1	D	140	TYR	3.1
1	B	432	LEU	3.0
1	A	425	LEU	2.9
1	D	224	GLY	2.9
1	D	229	GLY	2.8
1	B	419	LEU	2.8
1	C	395	LEU	2.7
1	D	230	THR	2.7
1	A	6	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	85	ALA	2.6
1	B	429	THR	2.6
1	C	44	ILE	2.6
1	A	42	ALA	2.5
1	C	365	SER	2.4
1	C	54	ILE	2.4
1	C	397	THR	2.4
1	C	428	SER	2.3
1	A	90	HIS	2.3
1	D	40	GLY	2.3
1	D	156	THR	2.3
1	B	54	ILE	2.3
1	C	438	GLU	2.3
1	A	102	ALA	2.2
1	D	157	TYR	2.3
1	A	433	HIS	2.2
1	D	148	VAL	2.2
1	D	185	VAL	2.2
1	D	392	ALA	2.2
1	D	389	THR	2.2
1	D	429	THR	2.2
1	D	186	TYR	2.2
1	A	228	LEU	2.2
1	C	372	PRO	2.2
1	C	374	PRO	2.2
1	B	412	GLN	2.2
1	D	225	ASP	2.2
1	B	386	ALA	2.1
1	C	377	ALA	2.1
1	D	23	GLN	2.1
1	D	129	GLN	2.1
1	D	191	GLN	2.1
1	C	376	ASN	2.1
1	C	45	GLN	2.1
1	B	414	LEU	2.1
1	A	73	ALA	2.0
1	B	396	ALA	2.0
1	D	136	GLN	2.0
1	A	303	ALA	2.0
1	D	146	ALA	2.0
1	C	337	TYR	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	GOL	D	453	6/6	0.82	0.19	70,70,71,72	0
3	GOL	C	455	6/6	0.84	0.17	71,72,72,73	0
3	GOL	B	453	6/6	0.90	0.14	60,61,62,64	0
2	CL	C	454	1/1	0.93	0.10	51,51,51,51	0
2	CL	B	454	1/1	0.94	0.12	82,82,82,82	0
3	GOL	C	453	6/6	0.95	0.09	50,52,53,55	0
2	CL	A	453	1/1	0.97	0.13	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.