



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:00 PM GMT

PDB ID : 1RLT
Title : Transition State Analogue of ybiV from E. coli K12
Authors : Roberts, A.; Lee, S.Y.; McCullagh, E.; Silversmith, R.E.; Wemmer, D.E.
Deposited on : 2003-11-26
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

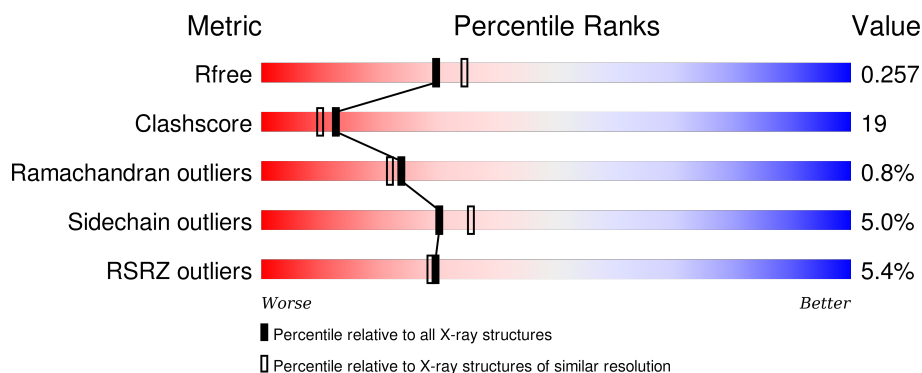
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	271	<div> <div>%</div> <div>67% 29% ..</div> </div>
1	B	271	<div> <div>6%</div> <div>65% 30% ..</div> </div>
1	C	271	<div> <div>13%</div> <div>60% 35% ..</div> </div>
1	D	271	<div> <div>%</div> <div>67% 29% ..</div> </div>

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	ACT	A	800	-	-	-	X
4	AF3	A	801	-	-	-	X
4	AF3	D	804	-	-	-	X
5	GOL	C	759	-	X	-	X
5	GOL	D	758	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8949 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 Phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	B	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	C	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			
1	D	268	Total	C	N	O	S	0	0	0
			2129	1366	361	394	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	ENGINEERED	UNP P75792
A	267	TYR	SER	ENGINEERED	UNP P75792
B	2	ALA	SER	ENGINEERED	UNP P75792
B	267	TYR	SER	ENGINEERED	UNP P75792
C	2	ALA	SER	ENGINEERED	UNP P75792
C	267	TYR	SER	ENGINEERED	UNP P75792
D	2	ALA	SER	ENGINEERED	UNP P75792
D	267	TYR	SER	ENGINEERED	UNP P75792

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

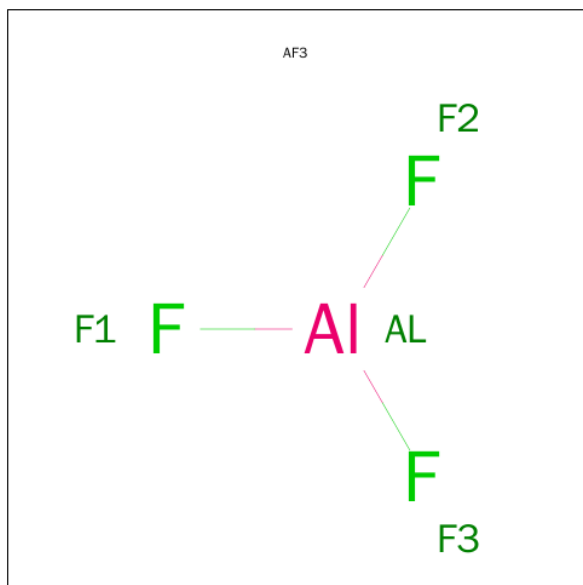
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 4 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		
4	B	1	Total	Al	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	Al	F	0	0
			4	1	3		
4	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

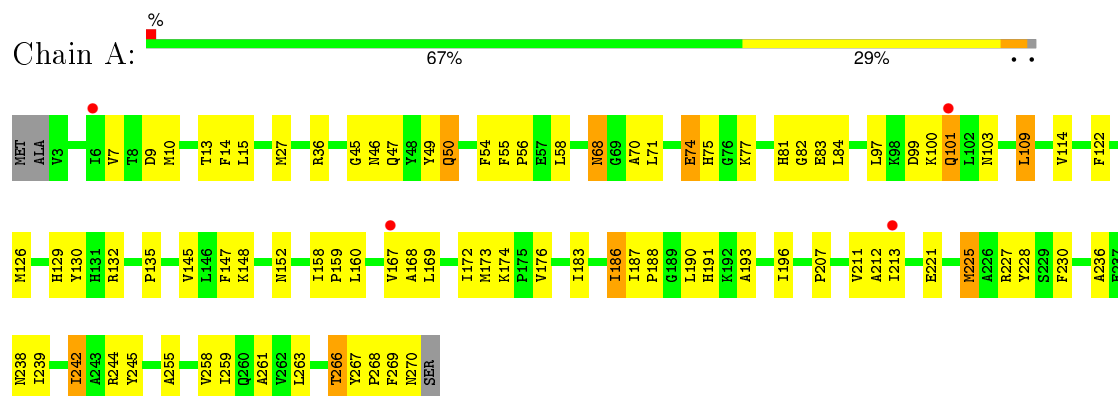
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	116	Total	O	0	0
			116	116		
6	B	111	Total	O	0	0
			111	111		
6	C	76	Total	O	0	0
			76	76		
6	D	94	Total	O	0	0
			94	94		

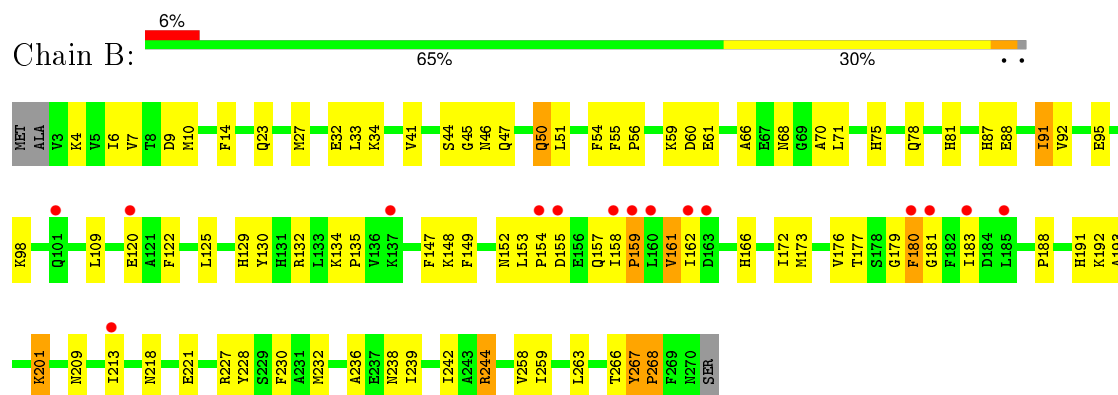
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

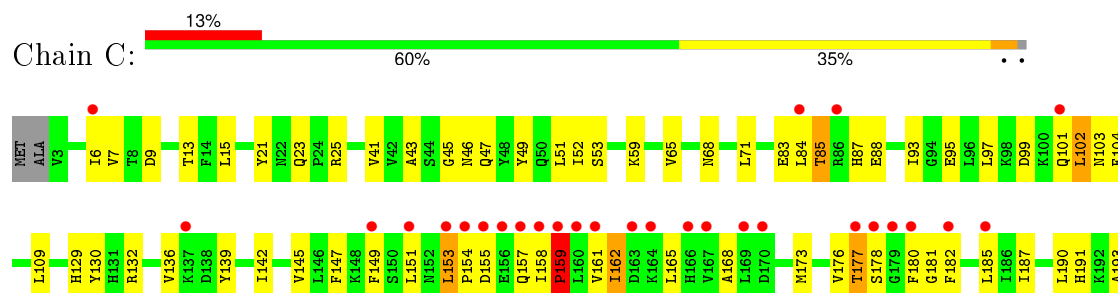
• Molecule 1: Phosphatase

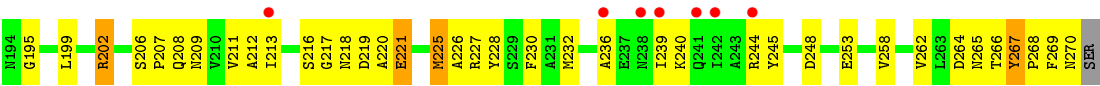


• Molecule 1: Phosphatase

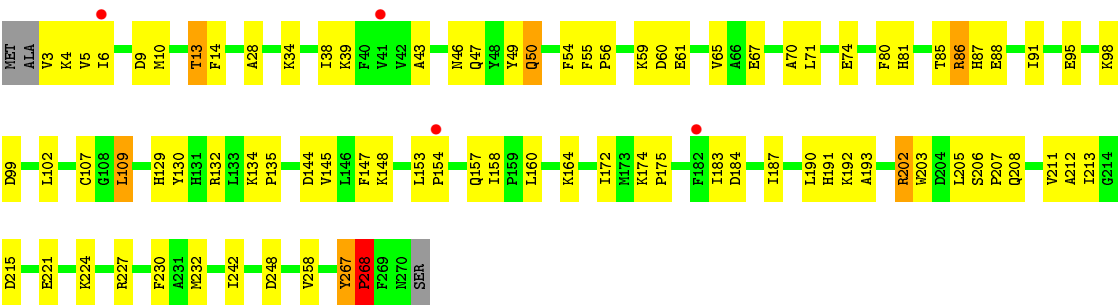


• Molecule 1: Phosphatase





● Molecule 1: Phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.76 Å 91.17 Å 183.85 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.20 20.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.93-2.20) 96.5 (20.05-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.19 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.264 0.216 , 0.257	Depositor DCC
R_{free} test set	6223 reflections (11.57%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61474 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8949	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, ACT, AF3

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	0.46	0/2174	0.74	3/2939 (0.1%)
1	B	0.48	1/2174 (0.0%)	0.82	3/2939 (0.1%)
1	C	0.45	0/2174	0.81	3/2939 (0.1%)
1	D	0.41	0/2174	0.81	2/2939 (0.1%)
All	All	0.45	1/8696 (0.0%)	0.79	11/11756 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	PRO	N-CD	-7.01	1.38	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	TYR	C-N-CD	-22.70	70.66	120.60
1	B	267	TYR	C-N-CD	-22.55	70.98	120.60
1	C	154	PRO	CA-N-CD	-15.42	89.92	111.50
1	C	267	TYR	C-N-CD	-13.43	91.05	120.60
1	D	267	TYR	C-N-CA	13.05	176.83	122.00
1	B	267	TYR	C-N-CA	12.73	175.48	122.00
1	A	267	TYR	C-N-CD	-11.20	95.95	120.60
1	C	267	TYR	C-N-CA	9.09	160.18	122.00
1	A	267	TYR	C-N-CA	7.51	153.53	122.00
1	B	159	PRO	CA-N-CD	-5.38	103.96	111.50
1	A	9	ASP	CB-CG-OD1	-5.09	113.72	118.30

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	2129	0	2119	75	0
1	B	2129	0	2119	80	0
1	C	2129	0	2119	103	0
1	D	2129	0	2119	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	3	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
4	C	4	0	0	0	0
4	D	4	0	0	1	0
5	C	6	0	4	1	0
5	D	6	0	4	4	0
6	A	116	0	0	4	0
6	B	111	0	0	3	0
6	C	76	0	0	5	0
6	D	94	0	0	4	0
All	All	8949	0	8487	331	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 (331) 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:153:LEU:HD13	1:C:161:VAL:HG21	1.24	1.09
1:A:84:LEU:HD21	1:A:187:ILE:HD11	1.38	1.06
1:C:245:TYR:CE2	1:C:268:PRO:HB3	1.91	1.05
1:C:153:LEU:HD12	1:C:161:VAL:HG11	1.37	1.02
1:B:236:ALA:HB3	1:B:239:ILE:HD13	1.42	1.02
1:C:153:LEU:CD1	1:C:161:VAL:HG21	1.91	0.99
1:C:6:ILE:HD13	1:C:211:VAL:HB	1.49	0.95
1:D:158:ILE:HG23	1:D:183:ILE:HD11	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:HD12	1:B:172:ILE:HD12	1.47	0.93
1:B:6:ILE:HD13	1:B:259:ILE:HD13	1.51	0.91
1:C:104:PHE:HB3	1:C:151:LEU:HD23	1.52	0.91
1:C:195:GLY:O	6:C:880:HOH:O	1.88	0.90
1:C:178:SER:HG	5:C:759:GOL:HO3	0.90	0.89
1:B:87:HIS:O	1:B:91:ILE:HG22	1.73	0.86
1:C:104:PHE:HB3	1:C:151:LEU:CD2	2.04	0.86
1:A:84:LEU:CD2	1:A:187:ILE:HD11	2.06	0.86
1:B:6:ILE:HG21	1:B:259:ILE:HD11	1.56	0.85
1:A:238:ASN:O	1:A:242:ILE:HD13	1.77	0.85
1:D:6:ILE:HD13	1:D:211:VAL:HB	1.55	0.84
1:A:103:ASN:HD22	1:A:152:ASN:HD22	1.23	0.84
1:A:261:ALA:HA	1:A:266:THR:HG23	1.57	0.84
1:A:255:ALA:O	1:A:259:ILE:HD13	1.78	0.83
1:D:213:ILE:HD11	1:D:258:VAL:HG11	1.59	0.83
1:C:83:GLU:HG3	1:C:145:VAL:HG13	1.61	0.82
1:A:174:LYS:O	1:A:186:ILE:HD13	1.78	0.82
1:C:202:ARG:HH11	1:C:202:ARG:HB3	1.42	0.82
1:B:158:ILE:HB	1:B:159:PRO:HD2	1.60	0.82
1:C:153:LEU:CD1	1:C:161:VAL:HG11	2.09	0.82
1:C:199:LEU:HG	6:C:880:HOH:O	1.80	0.81
1:C:85:THR:HG22	1:C:88:GLU:H	1.46	0.80
1:C:104:PHE:CB	1:C:151:LEU:HD23	2.13	0.79
1:C:213:ILE:HD11	1:C:258:VAL:HG11	1.63	0.79
1:C:136:VAL:HG11	1:C:142:ILE:HD11	1.64	0.78
1:C:208:GLN:HE22	1:C:227:ARG:HD3	1.49	0.77
1:C:180:PHE:HB2	1:C:182:PHE:CE1	2.19	0.77
1:D:267:TYR:CD2	1:D:268:PRO:HD3	2.20	0.76
1:B:6:ILE:CD1	1:B:259:ILE:HD13	2.16	0.74
1:C:173:MET:CE	1:C:185:LEU:O	2.34	0.74
1:B:6:ILE:HG21	1:B:259:ILE:CD1	2.17	0.74
1:C:177:THR:O	1:C:177:THR:HG22	1.87	0.74
1:B:213:ILE:HD11	1:B:258:VAL:HG11	1.70	0.72
1:A:213:ILE:HD11	1:A:258:VAL:HG11	1.71	0.72
1:B:221:GLU:HG2	6:B:835:HOH:O	1.89	0.72
1:B:201:LYS:HA	1:B:201:LYS:HE2	1.69	0.71
1:C:84:LEU:HD21	1:C:187:ILE:HG13	1.71	0.71
1:A:84:LEU:HD21	1:A:187:ILE:CD1	2.17	0.71
1:C:187:ILE:HB	1:C:190:LEU:HD12	1.71	0.71
1:B:91:ILE:HD13	1:B:91:ILE:C	2.10	0.71
1:C:158:ILE:HG22	1:C:159:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ASN:OD1	1:A:129:HIS:HD2	1.74	0.70
1:C:202:ARG:NH1	1:C:202:ARG:HB3	2.06	0.70
1:C:6:ILE:HD13	1:C:211:VAL:CB	2.20	0.70
1:D:9:ASP:HB3	1:D:13:THR:HG21	1.72	0.70
1:A:266:THR:OG1	6:A:920:HOH:O	2.08	0.69
1:B:213:ILE:CG2	1:B:232:MET:CE	2.70	0.69
1:C:136:VAL:HG11	1:C:142:ILE:CD1	2.22	0.69
1:A:169:LEU:O	1:A:172:ILE:HG12	1.92	0.69
1:C:245:TYR:CE2	1:C:268:PRO:CB	2.72	0.68
1:D:187:ILE:HB	1:D:190:LEU:HD12	1.76	0.68
1:C:159:PRO:O	1:C:162:ILE:HB	1.95	0.67
1:D:158:ILE:CG2	1:D:183:ILE:HD11	2.24	0.66
1:D:221:GLU:HG2	6:D:838:HOH:O	1.95	0.65
1:B:213:ILE:HG21	1:B:232:MET:HE3	1.77	0.65
1:A:191:HIS:CG	1:A:221:GLU:HG3	2.32	0.65
1:D:49:TYR:CG	1:D:132:ARG:HD3	2.33	0.64
1:C:153:LEU:HD12	1:C:161:VAL:CG1	2.23	0.64
1:A:109:LEU:HB2	1:A:145:VAL:HG13	1.77	0.64
1:C:6:ILE:HD11	1:C:262:VAL:HG21	1.80	0.63
1:D:9:ASP:HB3	1:D:13:THR:CG2	2.27	0.63
1:B:88:GLU:O	1:B:91:ILE:HG23	1.98	0.63
1:B:244:ARG:O	1:B:244:ARG:HD3	1.99	0.63
1:A:83:GLU:HB2	1:A:145:VAL:HG23	1.81	0.63
1:C:161:VAL:O	1:C:161:VAL:HG12	1.98	0.62
1:A:236:ALA:HB3	1:A:239:ILE:HD13	1.80	0.62
1:A:186:ILE:H	1:A:186:ILE:HD13	1.64	0.62
1:C:155:ASP:OD1	1:C:181:GLY:HA2	2.00	0.62
1:A:45:GLY:HA2	1:A:68:ASN:N	2.15	0.62
1:B:238:ASN:O	1:B:242:ILE:HG12	2.00	0.62
1:B:213:ILE:CG2	1:B:232:MET:HE3	2.30	0.61
1:C:25:ARG:NH1	1:C:253:GLU:OE1	2.33	0.61
1:B:213:ILE:CG2	1:B:232:MET:HE2	2.30	0.61
1:D:191:HIS:CE1	1:D:193:ALA:HB3	2.36	0.61
1:B:27:MET:HE1	6:B:827:HOH:O	2.01	0.61
1:D:99:ASP:OD2	1:D:102:LEU:HD13	2.01	0.61
1:C:177:THR:CG2	1:C:177:THR:O	2.49	0.60
1:A:83:GLU:HB2	1:A:145:VAL:CG2	2.31	0.60
1:C:158:ILE:HD11	1:C:181:GLY:HA2	1.83	0.60
1:B:179:GLY:HA3	6:B:857:HOH:O	2.02	0.60
1:C:245:TYR:CD2	1:C:268:PRO:HB3	2.36	0.59
1:A:103:ASN:HD22	1:A:152:ASN:ND2	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LEU:HD11	1:C:151:LEU:HD13	1.84	0.58
1:C:155:ASP:OD1	1:C:181:GLY:CA	2.50	0.58
1:B:158:ILE:CB	1:B:159:PRO:HD2	2.32	0.58
1:A:50:GLN:NE2	6:A:825:HOH:O	2.30	0.58
1:B:157:GLN:O	1:B:161:VAL:HG22	2.04	0.58
1:B:266:THR:O	1:B:267:TYR:C	2.39	0.58
1:C:7:VAL:HG22	1:C:41:VAL:HB	1.86	0.58
1:A:158:ILE:N	1:A:159:PRO:HD2	2.19	0.58
1:D:47:GLN:HB2	1:D:130:TYR:CD2	2.38	0.58
1:B:213:ILE:HG21	1:B:232:MET:CE	2.32	0.58
1:A:49:TYR:CD1	1:A:132:ARG:HD3	2.39	0.57
1:A:46:ASN:OD1	1:A:129:HIS:CD2	2.57	0.57
1:C:264:ASP:HB2	1:C:266:THR:HG23	1.86	0.57
1:B:50:GLN:HG2	1:B:129:HIS:O	2.04	0.57
1:B:162:ILE:O	1:B:166:HIS:HB2	2.04	0.57
1:B:91:ILE:HD12	1:B:172:ILE:CD1	2.27	0.57
1:C:180:PHE:HB2	1:C:182:PHE:CD1	2.40	0.57
1:B:91:ILE:HD13	1:B:92:VAL:N	2.20	0.57
1:B:155:ASP:OD2	1:B:181:GLY:HA2	2.04	0.57
1:C:187:ILE:HD13	6:C:812:HOH:O	2.05	0.57
1:D:224:LYS:HE2	1:D:242:ILE:HD12	1.87	0.57
1:C:236:ALA:O	1:C:240:LYS:HG3	2.05	0.57
1:B:213:ILE:CD1	1:B:230:PHE:HB2	2.35	0.56
1:A:70:ALA:O	1:A:81:HIS:HA	2.05	0.56
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.70	0.56
1:C:180:PHE:HB2	1:C:182:PHE:HE1	1.67	0.56
1:A:74:GLU:OE1	1:A:75:HIS:HB2	2.06	0.56
1:C:52:ILE:CG2	1:C:59:LYS:HG3	2.35	0.56
1:D:267:TYR:CG	1:D:268:PRO:HD3	2.41	0.56
1:A:158:ILE:HD11	1:A:183:ILE:HG23	1.88	0.56
1:D:160:LEU:O	1:D:164:LYS:HG3	2.05	0.56
1:A:122:PHE:CE1	1:A:152:ASN:HB2	2.41	0.56
1:C:155:ASP:HA	1:C:158:ILE:HD12	1.89	0.55
1:C:153:LEU:CD1	1:C:161:VAL:CG2	2.76	0.55
1:D:3:VAL:O	1:D:38:ILE:HD12	2.06	0.55
1:A:50:GLN:HG2	1:A:129:HIS:O	2.06	0.55
1:A:213:ILE:HD12	1:A:230:PHE:HB2	1.89	0.55
1:C:208:GLN:NE2	1:C:227:ARG:HD3	2.18	0.55
1:C:216:SER:HA	1:C:239:ILE:HG13	1.88	0.54
1:A:109:LEU:HB2	1:A:145:VAL:CG1	2.37	0.54
1:C:206:SER:H	1:C:209:ASN:HD22	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:THR:CG2	1:B:218:ASN:H	2.20	0.54
1:B:47:GLN:HB2	1:B:130:TYR:CD2	2.43	0.54
1:C:173:MET:HE2	1:C:185:LEU:O	2.05	0.53
1:C:85:THR:CG2	1:C:87:HIS:HB3	2.37	0.53
1:B:9:ASP:OD1	1:B:192:LYS:NZ	2.42	0.53
1:B:55:PHE:N	1:B:56:PRO:HD3	2.24	0.53
1:C:187:ILE:HD12	1:C:187:ILE:N	2.24	0.53
1:D:172:ILE:N	1:D:172:ILE:HD12	2.24	0.53
1:D:212:ALA:O	1:D:213:ILE:HD13	2.09	0.53
1:C:176:VAL:HG12	1:C:177:THR:N	2.24	0.53
1:D:153:LEU:N	1:D:153:LEU:HD23	2.24	0.53
1:C:93:ILE:HD12	1:C:139:TYR:HB3	1.91	0.53
1:B:239:ILE:N	1:B:239:ILE:HD12	2.24	0.52
1:A:212:ALA:O	1:A:213:ILE:HD13	2.08	0.52
1:A:261:ALA:HA	1:A:266:THR:CG2	2.35	0.52
1:A:213:ILE:CD1	1:A:258:VAL:HG11	2.39	0.52
1:B:10:MET:HB2	4:B:802:AF3:F2	2.00	0.52
1:D:130:TYR:CE1	5:D:758:GOL:O3	2.62	0.52
1:A:227:ARG:HD2	1:A:244:ARG:NH2	2.25	0.52
1:D:184:ASP:OD2	5:D:758:GOL:O1	2.27	0.52
1:B:153:LEU:HB2	1:B:183:ILE:HD12	1.92	0.52
1:B:236:ALA:HB3	1:B:239:ILE:CD1	2.28	0.52
1:A:245:TYR:CZ	1:A:268:PRO:HB3	2.45	0.52
1:D:59:LYS:HE3	1:D:60:ASP:OD1	2.10	0.52
1:B:122:PHE:CE1	1:B:152:ASN:HB2	2.44	0.51
1:C:207:PRO:HB3	1:C:225:MET:HE2	1.93	0.51
1:D:39:LYS:HD3	1:D:203:TRP:CZ2	2.46	0.51
1:B:129:HIS:CD2	1:B:180:PHE:CE2	2.99	0.51
1:A:212:ALA:C	1:A:213:ILE:HD13	2.31	0.51
1:C:178:SER:HB3	1:C:182:PHE:HB2	1.93	0.51
1:C:99:ASP:OD1	1:C:101:GLN:HG2	2.11	0.50
1:C:157:GLN:O	1:C:161:VAL:HG23	2.11	0.50
1:B:120:GLU:HA	1:B:120:GLU:OE1	2.10	0.50
1:A:49:TYR:CG	1:A:132:ARG:HD3	2.46	0.50
1:D:107:CYS:SG	1:D:148:LYS:HE2	2.52	0.50
1:A:191:HIS:ND1	1:A:221:GLU:HG3	2.27	0.50
1:C:93:ILE:HD11	1:C:149:PHE:HE2	1.77	0.50
1:C:49:TYR:CG	1:C:132:ARG:HD3	2.46	0.50
1:B:6:ILE:CD1	1:B:259:ILE:CD1	2.86	0.50
1:D:46:ASN:HB3	1:D:50:GLN:HG2	1.94	0.50
1:C:84:LEU:HD21	1:C:187:ILE:CG1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLN:HE21	1:B:51:LEU:N	2.10	0.50
1:D:9:ASP:OD2	1:D:13:THR:HG23	2.12	0.49
1:D:6:ILE:HD13	1:D:211:VAL:CB	2.37	0.49
1:A:45:GLY:HA2	1:A:68:ASN:H	1.74	0.49
1:B:227:ARG:HG3	1:B:228:TYR:CD1	2.47	0.49
1:B:172:ILE:HG22	1:B:173:MET:HG3	1.93	0.49
1:C:13:THR:HG23	1:C:232:MET:SD	2.52	0.49
1:D:213:ILE:CD1	1:D:230:PHE:HB2	2.42	0.49
1:B:213:ILE:HD12	1:B:230:PHE:HB2	1.93	0.49
1:D:5:VAL:HG23	1:D:205:LEU:HD23	1.93	0.49
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.78	0.49
1:C:52:ILE:HD12	1:C:53:SER:N	2.27	0.49
1:C:173:MET:HE2	1:C:185:LEU:C	2.32	0.49
1:D:13:THR:HB	1:D:232:MET:CG	2.42	0.49
1:A:176:VAL:HG22	1:A:186:ILE:HD12	1.95	0.49
1:A:167:VAL:HG13	1:A:168:ALA:N	2.28	0.49
1:A:213:ILE:CD1	1:A:230:PHE:HB2	2.43	0.49
1:A:27:MET:SD	1:A:58:LEU:HD11	2.53	0.49
1:B:213:ILE:CD1	1:B:258:VAL:HG11	2.42	0.48
1:D:43:ALA:HA	1:D:65:VAL:HB	1.95	0.48
1:A:47:GLN:HB2	1:A:130:TYR:CD2	2.49	0.48
1:B:155:ASP:CG	1:B:181:GLY:HA2	2.33	0.48
1:D:46:ASN:OD1	1:D:129:HIS:HD2	1.96	0.48
1:B:154:PRO:HA	1:B:181:GLY:O	2.12	0.48
1:C:244:ARG:HD3	1:C:245:TYR:CE1	2.48	0.48
1:A:221:GLU:HG2	6:A:817:HOH:O	2.12	0.48
1:D:95:GLU:HA	1:D:98:LYS:HD3	1.96	0.48
1:D:203:TRP:HB3	1:D:205:LEU:HD13	1.96	0.48
1:D:13:THR:OG1	1:D:14:PHE:N	2.47	0.48
1:D:221:GLU:H	1:D:221:GLU:CD	2.15	0.48
1:A:269:PHE:O	1:A:270:ASN:HB3	2.14	0.48
1:C:212:ALA:O	1:C:213:ILE:HD13	2.14	0.48
1:D:174:LYS:HA	1:D:175:PRO:HD3	1.74	0.48
1:B:78:GLN:NE2	1:B:81:HIS:HD2	2.12	0.47
1:A:160:LEU:C	1:A:160:LEU:HD13	2.34	0.47
1:C:9:ASP:HB3	1:C:13:THR:CB	2.44	0.47
1:A:99:ASP:C	1:A:101:GLN:H	2.17	0.47
1:D:13:THR:HB	1:D:232:MET:HG3	1.96	0.47
1:D:50:GLN:NE2	6:D:809:HOH:O	2.46	0.47
1:D:109:LEU:HB2	1:D:145:VAL:HB	1.97	0.47
1:D:213:ILE:CD1	1:D:258:VAL:HG11	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:OE1	1:B:263:LEU:HD13	2.14	0.47
1:C:95:GLU:HG2	1:C:168:ALA:HB1	1.96	0.47
1:D:86:ARG:HG3	1:D:86:ARG:NH1	2.29	0.47
1:B:191:HIS:CE1	1:B:193:ALA:HB3	2.50	0.47
1:B:51:LEU:HD12	1:B:66:ALA:HB2	1.96	0.47
1:D:154:PRO:HB2	1:D:157:GLN:HG2	1.97	0.47
1:C:248:ASP:HB2	6:C:821:HOH:O	2.15	0.46
1:C:153:LEU:CD1	1:C:161:VAL:CG1	2.89	0.46
1:A:55:PHE:N	1:A:56:PRO:HD3	2.30	0.46
1:D:144:ASP:OD2	1:D:145:VAL:N	2.48	0.46
1:B:33:LEU:HD23	1:B:263:LEU:HD21	1.97	0.46
1:B:88:GLU:O	1:B:92:VAL:HG23	2.15	0.46
1:C:102:LEU:HD22	1:C:103:ASN:N	2.31	0.46
1:D:9:ASP:OD1	1:D:192:LYS:NZ	2.48	0.46
1:B:7:VAL:HG22	1:B:41:VAL:HB	1.97	0.46
1:D:34:LYS:HE2	1:D:61:GLU:OE1	2.15	0.46
1:C:47:GLN:HB2	1:C:130:TYR:CD2	2.51	0.46
1:C:213:ILE:CD1	1:C:258:VAL:HG11	2.40	0.46
1:A:245:TYR:CE2	1:A:268:PRO:HB3	2.51	0.46
1:C:46:ASN:HB2	1:C:51:LEU:HD21	1.97	0.45
1:B:23:GLN:O	1:B:27:MET:HG2	2.17	0.45
1:C:191:HIS:CG	1:C:221:GLU:HG3	2.51	0.45
1:A:36:ARG:NH1	1:A:263:LEU:HA	2.31	0.45
1:A:84:LEU:CD2	1:A:187:ILE:CD1	2.84	0.45
1:D:49:TYR:CD1	1:D:132:ARG:HD3	2.51	0.45
1:C:220:ALA:HB3	1:C:221:GLU:OE1	2.16	0.45
1:B:54:PHE:C	1:B:56:PRO:HD3	2.37	0.45
1:D:4:LYS:HA	1:D:38:ILE:HD12	1.98	0.45
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.80	0.45
1:A:207:PRO:HB3	1:A:225:MET:HE2	1.98	0.45
1:A:13:THR:HG22	1:A:14:PHE:N	2.32	0.45
1:A:261:ALA:CA	1:A:266:THR:HG23	2.38	0.45
1:A:126:MET:HA	1:A:126:MET:CE	2.47	0.45
1:A:160:LEU:HA	6:A:863:HOH:O	2.18	0.45
1:D:208:GLN:O	1:D:227:ARG:HD3	2.16	0.45
1:D:85:THR:OG1	1:D:88:GLU:HG3	2.17	0.44
1:C:211:VAL:HG22	1:C:228:TYR:HB2	2.00	0.44
1:B:95:GLU:OE2	1:B:98:LYS:HD2	2.18	0.44
1:B:158:ILE:CB	1:B:159:PRO:CD	2.94	0.44
1:A:54:PHE:C	1:A:56:PRO:HD3	2.38	0.44
1:D:87:HIS:O	1:D:91:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PHE:CZ	1:A:268:PRO:HG3	2.52	0.44
1:B:10:MET:HE1	1:B:14:PHE:CD2	2.52	0.44
1:A:7:VAL:HG11	1:A:196:ILE:HD11	1.99	0.44
1:C:265:ASN:O	1:C:270:ASN:HB3	2.18	0.44
1:A:158:ILE:HD11	1:A:183:ILE:HG12	1.99	0.44
1:D:130:TYR:OH	5:D:758:GOL:O3	2.34	0.44
1:A:191:HIS:CE1	1:A:193:ALA:HB3	2.52	0.44
1:A:211:VAL:HG22	1:A:228:TYR:HB2	2.00	0.44
1:B:213:ILE:HD13	1:B:230:PHE:HB2	2.00	0.44
1:B:45:GLY:HA2	1:B:68:ASN:H	1.82	0.44
1:C:267:TYR:CD2	1:C:267:TYR:C	2.90	0.43
1:D:54:PHE:C	1:D:56:PRO:HD3	2.38	0.43
1:D:55:PHE:N	1:D:56:PRO:HD3	2.33	0.43
1:D:132:ARG:HG2	6:D:816:HOH:O	2.18	0.43
1:B:134:LYS:HA	1:B:135:PRO:HD3	1.90	0.43
1:A:230:PHE:HZ	1:A:268:PRO:CG	2.31	0.43
1:C:177:THR:HG23	6:C:879:HOH:O	2.18	0.43
1:C:9:ASP:HB3	1:C:13:THR:OG1	2.18	0.43
1:B:70:ALA:O	1:B:81:HIS:HA	2.19	0.43
1:A:82:GLY:O	1:A:83:GLU:HB3	2.19	0.43
1:B:176:VAL:HG22	1:B:177:THR:N	2.33	0.43
1:D:206:SER:O	1:D:208:GLN:N	2.51	0.43
1:D:67:GLU:HB2	1:D:70:ALA:HB3	2.01	0.43
1:D:80:PHE:CG	1:D:81:HIS:N	2.87	0.43
1:B:45:GLY:HA2	1:B:68:ASN:N	2.34	0.42
1:C:52:ILE:HB	1:C:59:LYS:HG3	2.00	0.42
1:B:4:LYS:HG2	1:B:209:ASN:HB3	2.00	0.42
1:B:34:LYS:HE2	1:B:61:GLU:OE1	2.19	0.42
1:B:152:ASN:O	1:B:153:LEU:HD23	2.19	0.42
1:D:10:MET:HB2	4:D:804:AF3:F2	2.10	0.42
1:C:45:GLY:HA2	1:C:68:ASN:H	1.85	0.42
1:C:217:GLY:C	1:C:219:ASP:H	2.22	0.42
1:A:259:ILE:N	1:A:259:ILE:HD12	2.34	0.42
1:B:46:ASN:OD1	1:B:129:HIS:HD2	2.01	0.42
1:B:148:LYS:HG2	1:B:149:PHE:N	2.34	0.42
1:C:104:PHE:HB2	1:C:151:LEU:HD23	1.98	0.42
1:C:6:ILE:CD1	1:C:262:VAL:HG21	2.48	0.42
1:B:6:ILE:HD12	1:B:259:ILE:CD1	2.49	0.42
1:D:46:ASN:HB3	1:D:50:GLN:CG	2.50	0.42
1:C:213:ILE:CD1	1:C:230:PHE:HB2	2.49	0.42
1:C:191:HIS:CE1	1:C:193:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HB	1:A:190:LEU:HD12	2.01	0.42
1:C:46:ASN:OD1	1:C:129:HIS:HD2	2.03	0.42
1:B:59:LYS:NZ	1:B:60:ASP:OD1	2.49	0.42
1:D:74:GLU:OE2	1:D:202:ARG:HD2	2.20	0.42
1:C:102:LEU:CD2	1:C:103:ASN:N	2.83	0.41
1:C:173:MET:HE1	1:C:185:LEU:HB2	2.02	0.41
1:B:213:ILE:HG22	1:B:232:MET:CE	2.48	0.41
1:C:43:ALA:HA	1:C:65:VAL:HB	2.02	0.41
1:A:114:VAL:O	1:A:135:PRO:HA	2.20	0.41
1:A:77:LYS:HB3	1:A:77:LYS:HE2	1.79	0.41
1:C:208:GLN:HA	1:C:227:ARG:HB2	2.02	0.41
1:D:13:THR:HG22	1:D:215:ASP:HB3	2.02	0.41
1:A:10:MET:HB2	4:A:801:AF3:F2	2.10	0.41
1:C:161:VAL:CG1	1:C:161:VAL:O	2.67	0.41
1:D:28:ALA:HB3	6:D:856:HOH:O	2.20	0.41
1:B:173:MET:HA	1:B:188:PRO:HD3	2.03	0.41
1:C:225:MET:HE1	1:C:226:ALA:HA	2.03	0.41
1:D:206:SER:C	1:D:208:GLN:H	2.24	0.41
1:B:125:LEU:HD23	1:B:125:LEU:O	2.20	0.41
1:C:104:PHE:CB	1:C:151:LEU:CD2	2.82	0.41
1:D:86:ARG:HA	1:D:86:ARG:HD2	1.88	0.41
1:D:39:LYS:HD3	1:D:203:TRP:CE2	2.55	0.41
1:A:259:ILE:N	1:A:259:ILE:CD1	2.83	0.41
1:D:203:TRP:O	1:D:205:LEU:CD1	2.69	0.41
1:C:21:TYR:CE1	1:C:23:GLN:HG2	2.56	0.41
1:A:148:LYS:HA	1:A:173:MET:HE1	2.03	0.40
1:A:83:GLU:CB	1:A:145:VAL:CG2	2.99	0.40
1:C:52:ILE:HD12	1:C:52:ILE:C	2.42	0.40
1:A:173:MET:HA	1:A:188:PRO:HD3	2.03	0.40
1:D:134:LYS:HA	1:D:135:PRO:HD3	1.92	0.40
1:D:153:LEU:N	1:D:153:LEU:CD2	2.85	0.40
1:D:130:TYR:HE1	5:D:758:GOL:O3	2.02	0.40
1:C:158:ILE:HG22	1:C:159:PRO:CD	2.46	0.40
1:B:46:ASN:OD1	1:B:129:HIS:CD2	2.74	0.40
1:B:44:SER:HA	1:B:192:LYS:HE2	2.04	0.40
1:D:70:ALA:O	1:D:81:HIS:HA	2.21	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	266/271 (98%)	254 (96%)	11 (4%)	1 (0%)	39	42
1	B	266/271 (98%)	248 (93%)	16 (6%)	2 (1%)	24	22
1	C	266/271 (98%)	244 (92%)	19 (7%)	3 (1%)	17	14
1	D	266/271 (98%)	252 (95%)	12 (4%)	2 (1%)	24	22
All	All	1064/1084 (98%)	998 (94%)	58 (6%)	8 (1%)	24	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	PRO
1	D	268	PRO
1	A	100	LYS
1	C	218	ASN
1	C	159	PRO
1	B	161	VAL
1	C	153	LEU
1	D	207	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	228/230 (99%)	215 (94%)	13 (6%)	25	29
1	B	228/230 (99%)	218 (96%)	10 (4%)	35	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	228/230 (99%)	214 (94%)	14 (6%)	23	26
1	D	228/230 (99%)	219 (96%)	9 (4%)	39	48
All	All	912/920 (99%)	866 (95%)	46 (5%)	30	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	50	GLN
1	A	68	ASN
1	A	71	LEU
1	A	74	GLU
1	A	97	LEU
1	A	101	GLN
1	A	109	LEU
1	A	147	PHE
1	A	186	ILE
1	A	225	MET
1	A	242	ILE
1	A	266	THR
1	B	50	GLN
1	B	71	LEU
1	B	75	HIS
1	B	91	ILE
1	B	109	LEU
1	B	132	ARG
1	B	147	PHE
1	B	180	PHE
1	B	201	LYS
1	B	244	ARG
1	C	15	LEU
1	C	71	LEU
1	C	85	THR
1	C	97	LEU
1	C	102	LEU
1	C	109	LEU
1	C	147	PHE
1	C	159	PRO
1	C	162	ILE
1	C	177	THR
1	C	202	ARG

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Mol	Chain	Res	Type
1	C	221	GLU
1	C	225	MET
1	C	269	PHE
1	D	13	THR
1	D	50	GLN
1	D	71	LEU
1	D	86	ARG
1	D	109	LEU
1	D	147	PHE
1	D	202	ARG
1	D	248	ASP
1	D	268	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	101	GLN
1	A	129	HIS
1	A	152	ASN
1	A	209	ASN
1	B	50	GLN
1	B	78	GLN
1	B	129	HIS
1	B	208	GLN
1	C	46	ASN
1	C	129	HIS
1	C	208	GLN
1	C	209	ASN
1	D	50	GLN
1	D	101	GLN
1	D	129	HIS
1	D	131	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	ACT	A	800	-	1,3,3	1.47	0	0,3,3	0.00	-
4	AF3	A	801	1,2,6	0,3,3	0.00	-	0,3,3	0.00	-
4	AF3	B	802	1,2,6	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	C	759	1	5,5,5	5.59	5 (100%)	5,5,5	5.84	3 (60%)
4	AF3	C	803	1,2,6	0,3,3	0.00	-	0,3,3	0.00	-
5	GOL	D	758	-	5,5,5	4.88	5 (100%)	5,5,5	5.58	3 (60%)
4	AF3	D	804	1,2,6	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	800	-	-	0/0/0/0	0/0/0/0
4	AF3	A	801	1,2,6	-	0/0/0/0	0/0/0/0
4	AF3	B	802	1,2,6	-	0/0/0/0	0/0/0/0
5	GOL	C	759	1	-	0/4/4/4	0/0/0/0
4	AF3	C	803	1,2,6	-	0/0/0/0	0/0/0/0
5	GOL	D	758	-	-	0/4/4/4	0/0/0/0
4	AF3	D	804	1,2,6	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	759	GOL	C3-C2	-9.45	1.16	1.52
5	D	758	GOL	C3-C2	-8.86	1.18	1.52
5	C	759	GOL	O2-C2	-5.80	1.26	1.43
5	D	758	GOL	C1-C2	-3.34	1.39	1.52
5	D	758	GOL	O2-C2	-2.86	1.34	1.43
5	C	759	GOL	C1-C2	-2.55	1.42	1.52
5	D	758	GOL	O3-C3	2.13	1.51	1.42
5	C	759	GOL	O3-C3	2.15	1.51	1.42
5	D	758	GOL	O1-C1	4.09	1.60	1.42
5	C	759	GOL	O1-C1	4.70	1.62	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	759	GOL	C3-C2-C1	2.42	120.61	111.12
5	D	758	GOL	O1-C1-C2	3.08	125.14	110.18
5	C	759	GOL	O2-C2-C3	5.14	132.24	108.65
5	D	758	GOL	O2-C2-C3	6.54	138.65	108.65
5	D	758	GOL	O3-C3-C2	10.13	159.29	110.18
5	C	759	GOL	O3-C3-C2	11.65	166.68	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	AF3	1	0
4	B	802	AF3	1	0
5	C	759	GOL	1	0
5	D	758	GOL	4	0
4	D	804	AF3	1	0

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	268/271 (98%)	-0.07	4 (1%) 76 75	16, 31, 57, 75	0
1	B	268/271 (98%)	0.24	15 (5%) 28 27	20, 35, 79, 123	0
1	C	268/271 (98%)	0.54	35 (13%) 5 4	24, 41, 98, 144	0
1	D	268/271 (98%)	0.04	4 (1%) 76 75	21, 35, 61, 87	0
All	All	1072/1084 (98%)	0.19	58 (5%) 29 29	16, 36, 77, 144	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ASP	9.9
1	C	154	PRO	6.9
1	B	180	PHE	6.1
1	C	153	LEU	5.7
1	C	160	LEU	5.3
1	B	160	LEU	5.2
1	B	162	ILE	5.2
1	C	180	PHE	4.9
1	C	166	HIS	4.7
1	C	161	VAL	4.3
1	C	156	GLU	4.2
1	C	157	GLN	3.9
1	C	86	ARG	3.7
1	B	154	PRO	3.5
1	C	170	ASP	3.4
1	B	101	GLN	3.4
1	B	158	ILE	3.2
1	C	101	GLN	3.1
1	C	179	GLY	3.0
1	C	159	PRO	2.9
1	C	169	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	163	ASP	2.8
1	A	101	GLN	2.6
1	C	155	ASP	2.6
1	D	6	ILE	2.6
1	B	159	PRO	2.6
1	A	167	VAL	2.5
1	C	149	PHE	2.5
1	C	236	ALA	2.5
1	C	178	SER	2.4
1	C	6	ILE	2.4
1	C	182	PHE	2.4
1	A	6	ILE	2.3
1	C	137	LYS	2.3
1	C	164	LYS	2.3
1	A	213	ILE	2.3
1	B	183	ILE	2.3
1	D	154	PRO	2.3
1	B	120	GLU	2.3
1	C	239	ILE	2.2
1	C	244	ARG	2.2
1	B	181	GLY	2.2
1	B	137	LYS	2.2
1	C	185	LEU	2.2
1	B	155	ASP	2.2
1	C	167	VAL	2.2
1	C	238	ASN	2.2
1	C	242	ILE	2.1
1	B	213	ILE	2.1
1	C	241	GLN	2.1
1	B	185	LEU	2.1
1	C	84	LEU	2.1
1	C	158	ILE	2.1
1	C	213	ILE	2.1
1	C	177	THR	2.0
1	C	151	LEU	2.0
1	D	182	PHE	2.0
1	D	41	VAL	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	A	800	4/4	0.93	0.27	19.08	28,30,31,31	0
4	AF3	A	801	4/4	0.93	0.26	8.28	41,43,44,46	0
5	GOL	C	759	6/6	0.74	0.43	3.72	43,46,46,48	0
4	AF3	D	804	4/4	0.84	0.18	2.18	54,55,55,56	0
4	AF3	C	803	4/4	0.91	0.22	1.84	58,58,58,58	0
4	AF3	B	802	4/4	0.91	0.20	1.77	51,52,52,52	0
5	GOL	D	758	6/6	0.76	0.22	1.68	28,34,35,37	0
2	MG	A	805	1/1	0.94	0.11	-0.17	25,25,25,25	0
2	MG	B	806	1/1	0.94	0.08	-0.90	37,37,37,37	0
2	MG	C	807	1/1	0.81	0.10	-1.18	39,39,39,39	0
2	MG	D	808	1/1	0.95	0.07	-1.33	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.