



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:19 PM GMT

PDB ID : 3D5Q
Title : Crystal Structure of 11b-HSD1 in Complex with Triazole Inhibitor
Authors : Wang, Z.; Liu, J.; Sudom, A.; Walker, N.P.C.
Deposited on : 2008-05-16
Resolution : 2.55 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

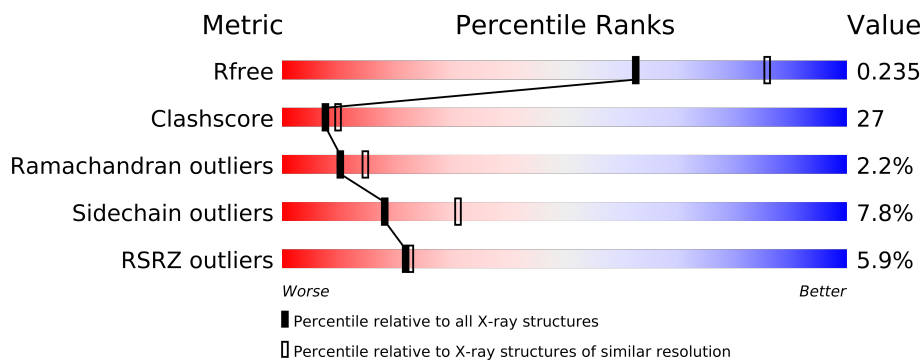
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	272	
1	B	272	
1	C	272	
1	D	272	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8311 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	1	0
			2039	1300	344	379	16			
1	B	264	Total	C	N	O	S	0	5	0
			2042	1306	343	378	15			
1	C	253	Total	C	N	O	S	0	1	0
			1946	1242	329	361	14			
1	D	257	Total	C	N	O	S	0	1	0
			1976	1261	333	366	16			

There are 16 discrepancies between the modelled and reference sequences:

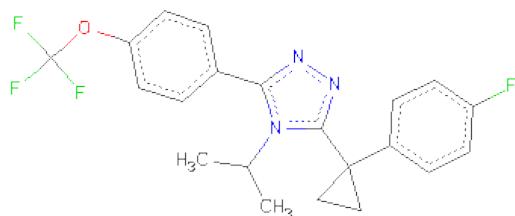
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[1-(4-FLUOROPHENYL)CYCLOPROPYL]-4-(1-METHYLETHYL)-5-[4-(TRIFLUOROMETHOXY)PHENYL]-4H-1,2,4-TRIAZOLE (three-letter code: T30) (formula: C₂₁H₁₉F₄N₃O).



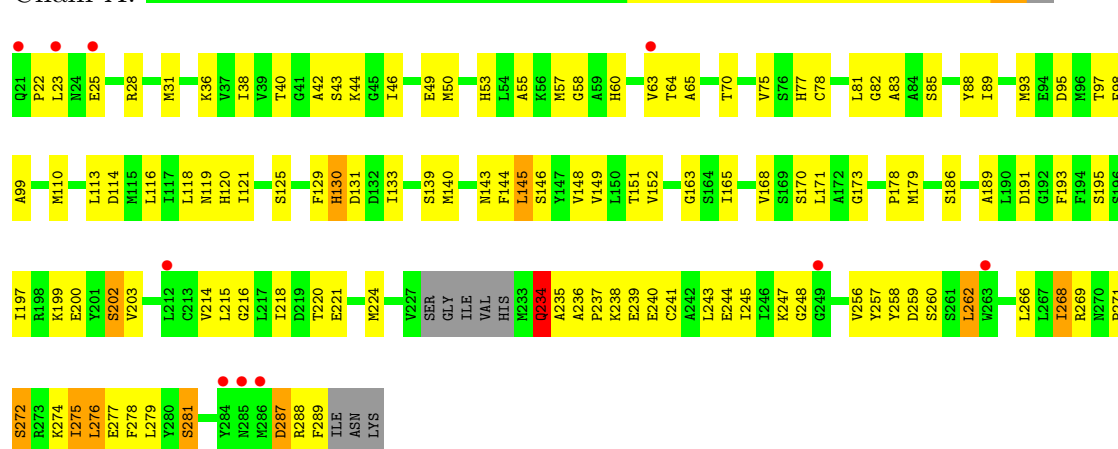
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 21	F 4	N 3	O 1	0	0
3	B	1	Total 29	C 21	F 4	N 3	O 1	0	0
3	C	1	Total 29	C 21	F 4	N 3	O 1	0	0
3	D	1	Total 29	C 21	F 4	N 3	O 1	0	0

3 Residue-property plots

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 ($RSRZ > 2$). 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.

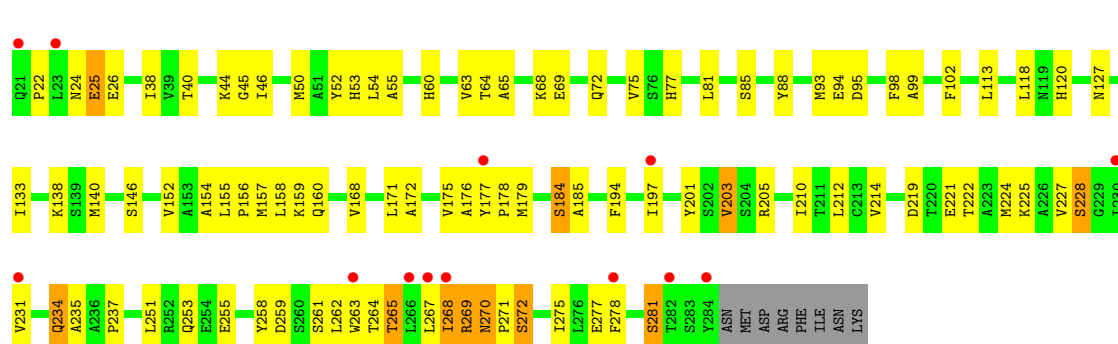
- Molecule 1: Corticosteroid 11-beta-dehydrogenaseisozyme 1

Chain A:



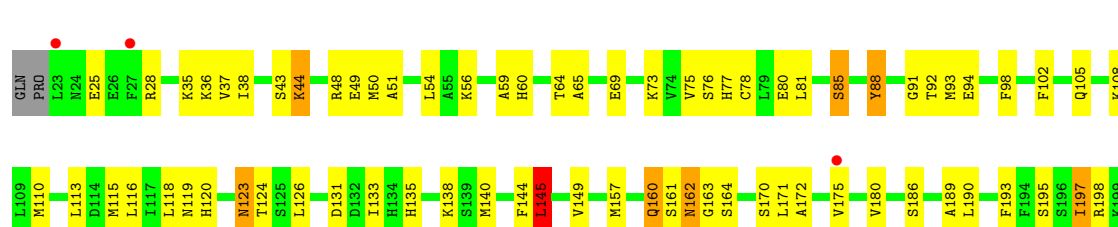
- Molecule 1: Corticosteroid 11-beta-dehydrogenaseisozyme 1

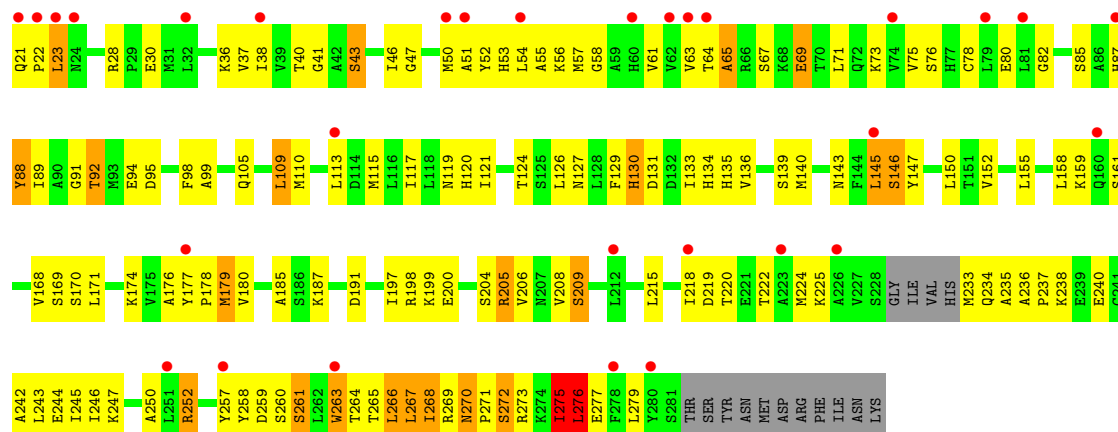
Chain B:



- Molecule 1: Corticosteroid 11-beta-dehydrogenaseisozyme 1

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.67Å 153.32Å 73.60Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 76.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.55) 99.7 (76.66-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.230 , 0.265 0.224 , 0.235	Depositor DCC
R_{free} test set	2045 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.6	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40748 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8311	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, T30

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	0.45	0/2077	0.63	1/2802 (0.0%)
1	B	0.47	0/2099	0.67	0/2836
1	C	0.49	0/1981	0.66	1/2673 (0.0%)
1	D	0.42	0/2012	0.65	1/2714 (0.0%)
All	All	0.46	0/8169	0.65	3/11025 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	CA-CB-CG	-5.69	102.22	115.30
1	A	145	LEU	CA-CB-CG	-5.42	102.85	115.30
1	D	276	LEU	CA-CB-CG	-5.27	103.18	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2039	0	2078	96	0
1	B	2042	0	2096	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1946	0	1993	95	0
1	D	1976	0	2025	175	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
3	A	29	0	19	5	0
3	B	29	0	19	5	0
3	C	29	0	19	2	0
3	D	29	0	19	6	0
All	All	8311	0	8368	457	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (457) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:124:THR:HG22	1:D:135:HIS:CE1	1.61	1.35
1:D:273:ARG:HA	1:D:276:LEU:CD1	1.73	1.17
1:D:124:THR:HG22	1:D:135:HIS:NE2	1.63	1.14
1:D:219:ASP:OD1	1:D:237:PRO:HA	1.47	1.13
1:D:124:THR:CG2	1:D:135:HIS:CE1	2.39	1.05
1:D:269:ARG:HH21	1:D:269:ARG:HB2	1.20	1.04
1:D:219:ASP:HA	1:D:224:MET:CE	1.87	1.03
1:D:219:ASP:HA	1:D:224:MET:HE3	1.35	1.03
1:D:269:ARG:NH2	1:D:269:ARG:HB2	1.73	1.03
1:D:273:ARG:CA	1:D:276:LEU:HD11	1.88	1.02
1:D:264:THR:O	1:D:267:LEU:HD12	1.61	1.00
1:D:92:THR:CG2	1:D:94:GLU:HB2	1.91	1.00
1:D:264:THR:O	1:D:268:ILE:HG23	1.62	0.98
1:D:261:SER:O	1:D:265:THR:HG23	1.62	0.98
1:A:171:LEU:HD12	3:A:293:T30:H22	1.46	0.97
1:D:272:SER:O	1:D:276:LEU:HD21	1.64	0.97
1:D:273:ARG:HA	1:D:276:LEU:HD11	0.97	0.95
1:D:92:THR:HG23	1:D:94:GLU:H	1.35	0.91
1:C:224:MET:HA	1:C:224:MET:HE2	1.52	0.90
1:B:267:LEU:HD23	1:B:267:LEU:H	1.37	0.90
1:A:272:SER:O	1:A:276:LEU:HD23	1.73	0.89
1:A:224:MET:CE	1:A:235:ALA:HB2	2.03	0.88
3:A:293:T30:H16B	3:A:293:T30:C20	2.04	0.88
1:A:28:ARG:O	1:A:31:MET:HG3	1.72	0.87
1:D:261:SER:HB3	1:D:264:THR:HG23	1.56	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:MET:HA	1:B:140:MET:HE3	1.57	0.87
1:B:46:ILE:HG22	1:B:50:MET:CE	2.04	0.87
1:C:269:ARG:NH1	1:C:274:LYS:HG3	1.89	0.86
1:D:252:ARG:HH11	1:D:252:ARG:CG	1.89	0.85
1:D:124:THR:CG2	1:D:135:HIS:NE2	2.39	0.84
1:B:194:PHE:CD2	1:B:197[A]:ILE:HD11	2.12	0.84
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.61	0.83
1:D:269:ARG:HH21	1:D:269:ARG:CB	1.92	0.82
1:D:95:ASP:HB3	1:D:98:PHE:HB3	1.60	0.81
1:D:124:THR:HG22	1:D:135:HIS:HE1	1.43	0.81
1:D:105:GLN:NE2	1:D:109:LEU:HD13	1.95	0.81
1:B:22:PRO:HG3	1:B:253:GLN:HA	1.62	0.81
1:A:276:LEU:H	1:A:276:LEU:HD23	1.46	0.80
1:C:203:VAL:C	1:C:205:ARG:H	1.81	0.80
1:B:222:THR:HA	1:B:225:LYS:HD2	1.63	0.79
1:B:46:ILE:HG22	1:B:50:MET:HE2	1.64	0.78
1:A:38:ILE:HG13	1:A:113:LEU:HD11	1.65	0.78
1:D:243:LEU:HG	1:D:247:LYS:CE	2.14	0.77
3:B:1:T30:C15	3:B:1:T30:H16B	2.16	0.76
1:B:270:ASN:C	1:B:270:ASN:HD22	1.88	0.75
1:D:50:MET:HG2	1:D:242:ALA:HB1	1.66	0.75
1:C:124:THR:HG22	1:C:135:HIS:CE1	2.22	0.75
1:A:38:ILE:HG13	1:A:113:LEU:CD1	2.16	0.75
1:D:92:THR:HG21	1:D:94:GLU:HB2	1.67	0.74
1:D:252:ARG:HG3	1:D:252:ARG:HH11	1.52	0.74
1:B:194:PHE:HA	1:B:197[A]:ILE:HG12	1.68	0.74
1:A:224:MET:HE1	1:A:235:ALA:HB2	1.67	0.74
1:B:234:GLN:HE21	1:B:234:GLN:HA	1.50	0.74
1:C:124:THR:HG22	1:C:135:HIS:NE2	2.03	0.73
1:D:178:PRO:C	1:D:179:MET:HG2	2.06	0.73
1:C:44:LYS:HE2	2:C:3:NAP:H3B	1.70	0.73
1:B:268:ILE:HD12	1:B:268:ILE:O	1.89	0.73
1:D:257:TYR:CD2	1:D:268:ILE:HD11	2.25	0.72
1:D:124:THR:CG2	1:D:135:HIS:HE1	1.96	0.72
1:A:224:MET:HE3	1:A:235:ALA:CB	2.19	0.72
1:B:46:ILE:HG22	1:B:50:MET:HE1	1.72	0.72
1:A:197:ILE:HA	1:A:200:GLU:HB2	1.71	0.71
1:C:25:GLU:HG3	1:C:28:ARG:HH22	1.53	0.71
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.72	0.71
1:D:219:ASP:CA	1:D:224:MET:HE3	2.18	0.71
1:C:224:MET:HA	1:C:224:MET:CE	2.21	0.70
1:D:261:SER:OG	1:D:263:TRP:HD1	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:269:ARG:HH11	1:C:274:LYS:HG3	1.54	0.70
1:D:50:MET:CE	1:D:117:ILE:HG21	2.22	0.70
1:D:243:LEU:HG	1:D:247:LYS:HE2	1.73	0.70
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.74	0.70
1:A:130:HIS:N	1:A:130:HIS:ND1	2.40	0.70
3:D:1:T30:C15	3:D:1:T30:H16B	2.22	0.70
1:D:273:ARG:NE	1:D:277:GLU:OE1	2.21	0.69
1:D:36:LYS:HB3	1:D:110:MET:HE3	1.74	0.69
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.75	0.69
1:B:94:GLU:OE2	1:B:138:LYS:HE2	1.92	0.69
1:D:197:ILE:O	1:D:198:ARG:C	2.32	0.69
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.57	0.69
1:B:270:ASN:HD22	1:B:271:PRO:N	1.92	0.68
1:D:92:THR:HG23	1:D:94:GLU:HB2	1.74	0.68
1:A:257:TYR:CG	1:A:268:ILE:HG21	2.29	0.68
1:A:60:HIS:HD1	1:A:85:SER:HG	1.33	0.68
1:D:219:ASP:HA	1:D:224:MET:HE2	1.72	0.68
1:D:261:SER:HG	1:D:263:TRP:HD1	1.40	0.67
1:B:219:ASP:OD1	1:B:237:PRO:HA	1.94	0.67
1:D:50:MET:HE3	1:D:117:ILE:HG21	1.74	0.67
1:B:224:MET:HE2	1:B:235:ALA:CB	2.24	0.67
1:A:199:LYS:O	1:A:202:SER:HB3	1.94	0.67
1:C:123:ASN:HD22	1:C:124:THR:N	1.93	0.66
1:B:277:GLU:O	1:B:281:SER:HB2	1.94	0.66
1:C:119:ASN:ND2	2:C:3:NAP:H4D	2.11	0.66
1:A:287:ASP:C	1:A:289:PHE:H	1.99	0.66
1:B:22:PRO:HA	1:B:251:LEU:O	1.96	0.66
1:A:224:MET:HE3	1:A:235:ALA:HB2	1.74	0.66
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.76	0.66
1:D:69:GLU:O	1:D:73:LYS:HG3	1.95	0.66
1:D:261:SER:OG	1:D:263:TRP:CD1	2.48	0.65
3:A:293:T30:H16B	3:A:293:T30:C15	2.27	0.65
1:C:203:VAL:C	1:C:205:ARG:N	2.45	0.65
1:D:261:SER:HB3	1:D:264:THR:CG2	2.26	0.64
1:C:244:GLU:OE1	1:C:247:LYS:HD2	1.96	0.64
1:B:24:ASN:O	1:B:25:GLU:HB3	1.97	0.64
1:C:276:LEU:HD11	1:D:268:ILE:HA	1.78	0.64
1:D:120:HIS:CE1	1:D:146:SER:OG	2.51	0.64
1:D:92:THR:CG2	1:D:94:GLU:H	2.09	0.64
1:D:261:SER:O	1:D:265:THR:CG2	2.42	0.63
3:A:293:T30:H17A	3:A:293:T30:H20	1.79	0.63
1:D:204:SER:C	1:D:206:VAL:H	2.00	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:270:ASN:ND2	1:D:273:ARG:H	1.96	0.63
1:B:275:ILE:HD11	1:D:266:LEU:HB3	1.81	0.63
1:D:120:HIS:O	1:D:121:ILE:HG23	1.98	0.63
1:A:148:VAL:O	1:A:152:VAL:HG23	1.99	0.62
1:D:271:PRO:O	1:D:275:ILE:HG12	1.99	0.62
1:B:262:LEU:HA	1:B:265:THR:HG23	1.79	0.62
1:A:129:PHE:HB3	1:B:197[B]:ILE:HD11	1.80	0.62
1:D:37:VAL:HG11	1:D:54:LEU:HD13	1.82	0.62
1:A:53:HIS:HB3	1:A:57:MET:HE3	1.82	0.62
1:C:270:ASN:OD1	1:C:273:ARG:HB2	1.99	0.62
1:D:264:THR:HA	1:D:267:LEU:HD11	1.81	0.62
1:A:93:MET:HG2	2:A:1:NAP:H2A	1.82	0.61
1:B:221:GLU:O	1:B:225:LYS:HG3	2.00	0.61
1:B:259:ASP:HB3	1:B:265:THR:HG22	1.81	0.61
1:C:157:MET:O	1:C:160:GLN:HB3	2.00	0.61
1:B:77:HIS:CE1	1:B:81:LEU:HG	2.35	0.61
1:C:261:SER:O	1:C:265:THR:HG23	1.99	0.61
1:A:214:VAL:C	1:A:215:LEU:HD23	2.20	0.61
1:D:275:ILE:HG22	1:D:279:LEU:HD11	1.83	0.61
1:A:60:HIS:ND1	1:A:85:SER:OG	2.30	0.61
1:A:116:LEU:HD11	1:A:118:LEU:HD21	1.82	0.61
1:C:37:VAL:HG11	1:C:54:LEU:HD13	1.83	0.61
1:C:48:ARG:O	1:C:51:ALA:N	2.34	0.61
1:D:234:GLN:HG3	1:D:260:SER:HB2	1.82	0.60
1:D:180:VAL:O	1:D:180:VAL:HG23	2.01	0.60
1:B:224:MET:CE	1:B:235:ALA:CB	2.79	0.60
1:B:270:ASN:C	1:B:270:ASN:ND2	2.53	0.60
1:C:259:ASP:OD2	1:C:264:THR:HG21	2.00	0.60
1:C:60:HIS:HD1	1:C:85:SER:HG	1.49	0.60
1:A:53:HIS:HB3	1:A:57:MET:CE	2.32	0.60
1:A:278:PHE:HA	1:A:281:SER:HB3	1.84	0.60
1:A:262:LEU:HD13	1:A:266:LEU:HD23	1.84	0.60
1:C:144:PHE:HD1	1:C:190:LEU:HD23	1.67	0.60
1:A:257:TYR:CD2	1:A:268:ILE:HG21	2.36	0.60
1:D:252:ARG:NH1	1:D:252:ARG:CG	2.54	0.60
1:D:37:VAL:HG22	1:D:115:MET:HB3	1.83	0.60
1:D:273:ARG:CA	1:D:276:LEU:CD1	2.63	0.60
1:C:170:SER:HA	1:C:215:LEU:H	1.67	0.60
1:D:120:HIS:HE1	1:D:146:SER:OG	1.85	0.60
1:D:46:ILE:HG13	1:D:220:THR:HG21	1.84	0.59
1:C:77:HIS:HA	1:C:80:GLU:OE2	2.02	0.59
1:D:85:SER:HB2	1:D:87:HIS:HE1	1.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:276:LEU:HD21	1:D:268:ILE:HG22	1.85	0.59
1:D:130:HIS:CD2	1:D:131:ASP:HB2	2.37	0.59
1:D:270:ASN:HD22	1:D:273:ARG:H	1.51	0.59
1:C:123:ASN:HD22	1:C:124:THR:H	1.49	0.59
1:B:172:ALA:O	1:B:184:SER:OG	2.21	0.59
1:C:170:SER:HB2	2:C:3:NAP:H5N	1.85	0.59
1:C:126:LEU:HD12	1:C:226:ALA:O	2.03	0.58
1:D:28:ARG:HB3	1:D:30:GLU:OE2	2.04	0.58
1:B:38:ILE:HG13	1:B:113:LEU:CD1	2.34	0.58
1:D:270:ASN:HD22	1:D:270:ASN:C	2.07	0.58
1:B:140:MET:CA	1:B:140:MET:HE3	2.29	0.58
1:D:43:SER:HB3	1:D:65:ALA:CB	2.34	0.58
1:D:89:ILE:HD11	1:D:105:GLN:HG3	1.86	0.58
1:A:236:ALA:HB2	1:A:260:SER:HB3	1.85	0.58
1:D:197:ILE:O	1:D:200:GLU:N	2.37	0.57
1:C:94:GLU:OE2	1:C:138:LYS:HE2	2.04	0.57
1:A:49:GLU:HG3	1:A:238:LYS:HG3	1.85	0.57
1:D:113:LEU:HD23	1:D:158:LEU:HG	1.86	0.57
1:A:218:ILE:CG2	1:A:238:LYS:HA	2.35	0.57
1:B:237:PRO:HD2	1:B:258:TYR:OH	2.05	0.57
1:B:94:GLU:OE2	1:B:138:LYS:CE	2.52	0.56
1:D:264:THR:C	1:D:268:ILE:HG23	2.26	0.56
1:D:242:ALA:HA	1:D:245:ILE:HD12	1.86	0.56
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.86	0.56
1:D:264:THR:OG1	1:D:265:THR:N	2.35	0.56
1:D:50:MET:HG2	1:D:242:ALA:CB	2.35	0.56
1:C:217:LEU:HD11	1:C:224:MET:HE1	1.87	0.56
1:C:131:ASP:O	1:C:133:ILE:HD12	2.05	0.56
1:D:85:SER:HB2	1:D:87:HIS:CE1	2.41	0.55
1:D:50:MET:CE	1:D:117:ILE:CG2	2.84	0.55
1:D:276:LEU:HA	1:D:279:LEU:HB2	1.88	0.55
1:D:145:LEU:O	1:D:146:SER:C	2.44	0.55
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.87	0.55
1:B:224:MET:O	1:B:225:LYS:C	2.44	0.55
1:C:180:VAL:O	1:C:180:VAL:HG23	2.05	0.55
1:B:267:LEU:H	1:B:267:LEU:CD2	2.16	0.55
1:D:53:HIS:CE1	1:D:243:LEU:HB2	2.42	0.55
1:C:124:THR:CG2	1:C:135:HIS:CE1	2.90	0.55
1:C:69:GLU:O	1:C:73:LYS:HG2	2.07	0.55
1:C:116:LEU:HG	1:C:118:LEU:HD21	1.88	0.54
1:B:24:ASN:O	1:B:25:GLU:CB	2.56	0.54
1:A:120:HIS:HE1	1:A:146:SER:OG	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:PRO:O	1:B:179:MET:HG3	2.08	0.54
1:A:202:SER:OG	1:A:203:VAL:HG13	2.07	0.54
1:A:272:SER:O	1:A:276:LEU:CD2	2.51	0.53
1:D:105:GLN:HE21	1:D:109:LEU:HD13	1.71	0.53
1:A:272:SER:O	1:A:275:ILE:HB	2.08	0.53
1:D:199:LYS:HE3	1:D:277:GLU:HB3	1.89	0.53
3:B:1:T30:H2O	3:B:1:T30:H17A	1.90	0.53
1:C:164:SER:HG	1:C:209:SER:HG	1.49	0.53
1:B:194:PHE:HA	1:B:197[A]:ILE:CG1	2.37	0.53
1:C:38:ILE:HG13	1:C:113:LEU:HD11	1.91	0.53
1:B:38:ILE:HG13	1:B:113:LEU:HD11	1.91	0.53
1:D:204:SER:O	1:D:206:VAL:N	2.41	0.53
1:D:105:GLN:NE2	1:D:109:LEU:CD1	2.70	0.53
1:B:177:TYR:CD1	3:B:1:T30:F27	2.52	0.53
1:A:240:GLU:O	1:A:241:CYS:C	2.48	0.53
1:B:234:GLN:NE2	1:B:234:GLN:HA	2.23	0.52
1:D:234:GLN:HE21	1:D:235:ALA:H	1.57	0.52
1:A:271:PRO:HA	1:A:274:LYS:HD2	1.90	0.52
1:D:267:LEU:O	1:D:269:ARG:O	2.28	0.52
1:D:268:ILE:HD12	1:D:268:ILE:O	2.09	0.52
1:B:127:ASN:O	1:B:179:MET:HA	2.10	0.52
1:A:58:GLY:HA2	1:A:82:GLY:O	2.10	0.52
1:C:50:MET:HG2	1:C:242:ALA:HB1	1.90	0.52
1:D:171:LEU:CD1	3:D:1:T30:H22	2.39	0.52
1:D:105:GLN:HE22	1:D:109:LEU:HD13	1.70	0.52
1:A:98:PHE:O	1:A:99:ALA:C	2.44	0.52
1:D:246:ILE:O	1:D:247:LYS:C	2.48	0.52
1:A:257:TYR:HE1	1:A:269:ARG:NH2	2.08	0.51
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.92	0.51
1:B:140:MET:HA	1:B:140:MET:CE	2.37	0.51
1:A:40:THR:HG1	1:A:119:ASN:H	1.56	0.51
1:D:204:SER:C	1:D:206:VAL:N	2.64	0.51
3:C:1:T30:C19	3:C:1:T30:H16B	2.41	0.51
1:B:72[B]:GLN:HG2	1:B:88:TYR:CE2	2.46	0.51
1:D:99:ALA:HB1	1:D:150:LEU:HD21	1.93	0.51
1:C:38:ILE:HG13	1:C:113:LEU:CD1	2.41	0.51
1:D:52:TYR:N	1:D:52:TYR:CD1	2.78	0.51
1:A:149:VAL:HG22	1:B:133:ILE:HD13	1.92	0.51
1:A:114:ASP:O	1:A:163:GLY:HA3	2.10	0.51
1:D:252:ARG:NH1	1:D:252:ARG:HG2	2.23	0.51
1:D:105:GLN:HE21	1:D:109:LEU:HD22	1.76	0.50
1:C:203:VAL:CG2	1:C:204:SER:N	2.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:37:VAL:HG21	1:C:54:LEU:HD22	1.93	0.50
1:B:178:PRO:C	1:B:179:MET:HG3	2.31	0.50
1:C:77:HIS:CD2	1:C:81:LEU:HD11	2.46	0.50
3:B:1:T30:C16	3:B:1:T30:C15	2.88	0.50
1:D:41:GLY:O	1:D:47:GLY:HA3	2.12	0.50
1:A:77:HIS:O	1:A:81:LEU:HG	2.10	0.50
1:D:55:ALA:C	1:D:57:MET:H	2.14	0.50
1:D:275:ILE:C	1:D:279:LEU:HG	2.32	0.50
1:D:50:MET:HE1	1:D:117:ILE:CG2	2.40	0.50
1:B:52:TYR:O	1:B:55:ALA:HB3	2.11	0.50
1:A:178:PRO:O	1:A:179:MET:HB2	2.12	0.50
1:D:177:TYR:CG	3:D:1:T30:H23	2.47	0.50
1:A:133:ILE:HD11	1:B:152:VAL:HG21	1.94	0.50
1:B:50:MET:O	1:B:54:LEU:HG	2.12	0.49
1:C:37:VAL:HG11	1:C:54:LEU:CD1	2.42	0.49
1:D:234:GLN:HE21	1:D:235:ALA:N	2.10	0.49
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.27	0.49
1:B:46:ILE:CG2	1:B:50:MET:HE1	2.41	0.49
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.48	0.49
1:C:270:ASN:OD1	1:C:273:ARG:CB	2.61	0.49
1:D:155:LEU:O	1:D:159:LYS:HG3	2.12	0.49
1:A:277:GLU:HG3	1:B:175:VAL:HB	1.94	0.49
1:B:201:TYR:CE2	1:B:210:ILE:HD11	2.47	0.49
1:C:198:ARG:NE	1:C:254:GLU:HG2	2.28	0.49
1:C:48:ARG:O	1:C:49:GLU:C	2.50	0.49
1:A:46:ILE:HG22	1:A:50:MET:CE	2.42	0.49
1:C:197:ILE:HD11	1:C:200:GLU:OE2	2.13	0.49
1:B:154:ALA:O	1:B:155:LEU:C	2.50	0.49
1:D:270:ASN:HD21	1:D:272:SER:HB2	1.77	0.49
1:A:191:ASP:OD1	1:A:195:SER:OG	2.27	0.49
1:D:206:VAL:HG12	1:D:208:VAL:HG23	1.94	0.48
3:D:1:T30:C15	3:D:1:T30:C16	2.91	0.48
1:C:197:ILE:HD11	1:D:129:PHE:HB3	1.94	0.48
1:A:139:SER:O	1:A:143:ASN:HB2	2.13	0.48
1:C:145:LEU:O	1:C:149:VAL:HG23	2.14	0.48
1:B:44:LYS:HG3	2:B:2:NAP:H3B	1.95	0.48
1:D:275:ILE:HB	1:D:276:LEU:H	1.52	0.48
1:D:233:MET:N	1:D:233:MET:SD	2.86	0.48
1:C:175:VAL:HG12	1:D:273:ARG:HG3	1.95	0.48
1:D:218:ILE:HD13	1:D:236:ALA:HB3	1.96	0.48
1:D:23:LEU:HG	1:D:252:ARG:HD2	1.96	0.48
1:C:118:LEU:HD23	1:C:118:LEU:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:209:SER:HB2	1:D:252:ARG:HG2	1.96	0.47
1:A:275:ILE:O	1:A:279:LEU:HG	2.15	0.47
1:D:178:PRO:O	1:D:179:MET:CG	2.61	0.47
1:C:203:VAL:HG23	1:C:204:SER:N	2.30	0.47
1:C:123:ASN:ND2	1:C:124:THR:N	2.61	0.47
1:D:53:HIS:HE1	1:D:243:LEU:HB2	1.79	0.47
1:C:164:SER:OG	1:C:209:SER:OG	2.24	0.47
1:A:88:TYR:C	1:A:89:ILE:HG13	2.34	0.47
1:A:171:LEU:CD2	1:A:268:ILE:HD11	2.45	0.47
1:B:94:GLU:OE2	1:B:138:LYS:NZ	2.46	0.47
1:C:133:ILE:H	1:C:133:ILE:HD12	1.80	0.47
1:C:207:ASN:OD1	1:C:252:ARG:NH2	2.47	0.47
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.48	0.47
3:A:293:T30:C16	3:A:293:T30:C15	2.92	0.47
1:A:237:PRO:HD2	1:A:258:TYR:OH	2.14	0.47
1:A:55:ALA:HB1	1:A:83:ALA:HB2	1.97	0.47
1:B:278:PHE:O	1:B:281:SER:HB3	2.14	0.47
1:A:260:SER:OG	1:A:260:SER:O	2.30	0.47
1:D:37:VAL:HG11	1:D:54:LEU:CD1	2.44	0.47
1:D:178:PRO:O	1:D:179:MET:HG2	2.15	0.47
1:D:46:ILE:HG13	1:D:220:THR:CG2	2.43	0.47
1:A:238:LYS:HE2	1:A:239:GLU:OE2	2.15	0.46
1:C:224:MET:CA	1:C:224:MET:CE	2.92	0.46
1:B:75:VAL:HG21	1:B:88:TYR:HD2	1.80	0.46
1:D:136:VAL:O	1:D:140[A]:MET:HG2	2.15	0.46
1:D:275:ILE:HG22	1:D:279:LEU:CD1	2.44	0.46
1:D:37:VAL:O	1:D:61:VAL:HA	2.14	0.46
1:C:171:LEU:HD12	1:C:216:GLY:HA2	1.98	0.46
1:B:271:PRO:O	1:B:275:ILE:HG12	2.15	0.46
1:B:22:PRO:CA	1:B:251:LEU:O	2.62	0.46
1:B:224:MET:CE	1:B:235:ALA:HB2	2.46	0.46
1:D:115:MET:HG2	1:D:117:ILE:HG13	1.97	0.46
1:B:268:ILE:HG23	1:B:269:ARG:N	2.31	0.46
1:A:234:GLN:O	1:A:260:SER:OG	2.24	0.46
1:D:271:PRO:O	1:D:272:SER:C	2.53	0.46
1:A:116:LEU:CD1	1:A:118:LEU:HD21	2.44	0.46
3:D:1:T30:H20	3:D:1:T30:H17A	1.96	0.46
1:A:287:ASP:C	1:A:289:PHE:N	2.66	0.46
1:C:115:MET:HA	1:C:164:SER:O	2.16	0.46
1:D:51:ALA:O	1:D:52:TYR:C	2.54	0.46
1:A:186:SER:O	1:A:189:ALA:HB3	2.16	0.46
1:D:92:THR:HG23	1:D:94:GLU:N	2.17	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:276:LEU:N	1:A:276:LEU:HD23	2.24	0.46
1:D:139:SER:O	1:D:143:ASN:HB2	2.15	0.45
1:B:68:LYS:O	1:B:72[A]:GLN:HG3	2.16	0.45
1:C:105:GLN:O	1:C:108:LYS:HB2	2.16	0.45
1:A:38:ILE:HG13	1:A:113:LEU:HD13	1.97	0.45
1:C:186:SER:O	1:C:189:ALA:HB3	2.17	0.45
1:A:268:ILE:CG2	1:A:269:ARG:N	2.80	0.45
1:D:36:LYS:HB3	1:D:110:MET:CE	2.44	0.45
1:A:244:GLU:O	1:A:245:ILE:C	2.55	0.45
1:A:278:PHE:HA	1:A:281:SER:CB	2.47	0.45
1:A:36:LYS:HD3	1:A:110:MET:O	2.16	0.45
1:D:127:ASN:O	1:D:179:MET:HA	2.16	0.45
1:B:201:TYR:HE2	1:B:210:ILE:HD11	1.82	0.45
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.79	0.45
1:B:171:LEU:HD21	1:B:268:ILE:HG12	1.99	0.45
1:C:149:VAL:HG22	1:D:133:ILE:HD13	1.99	0.45
1:D:52:TYR:HD1	1:D:52:TYR:N	2.14	0.45
1:C:195:SER:HB3	1:D:176:ALA:HB2	1.98	0.45
1:C:163:GLY:O	1:C:208:VAL:HA	2.17	0.45
1:D:63:VAL:HG23	1:D:71:LEU:HD22	1.98	0.45
1:D:95:ASP:HB3	1:D:98:PHE:CB	2.40	0.44
1:B:227:VAL:HB	1:B:231:VAL:HB	1.99	0.44
1:C:92:THR:OG1	1:C:94:GLU:HG3	2.17	0.44
1:C:88:TYR:CD1	1:C:88:TYR:C	2.89	0.44
1:B:98:PHE:O	1:B:99:ALA:C	2.54	0.44
1:B:64:THR:HB	1:B:102:PHE:CE1	2.52	0.44
1:D:187:LYS:NZ	2:D:4:NAP:O2D	2.41	0.44
1:C:35:LYS:O	1:C:59:ALA:HB1	2.18	0.44
1:C:105:GLN:HA	1:C:105:GLN:OE1	2.17	0.44
1:D:240:GLU:HB2	1:D:258:TYR:OH	2.16	0.44
1:C:119:ASN:HD21	2:C:3:NAP:H4D	1.82	0.44
1:D:155:LEU:HD12	1:D:155:LEU:HA	1.86	0.44
1:D:273:ARG:O	1:D:276:LEU:HD12	2.18	0.44
1:B:52:TYR:O	1:B:53:HIS:C	2.54	0.44
1:D:40:THR:O	1:D:41:GLY:C	2.54	0.44
1:D:133:ILE:O	1:D:134:HIS:C	2.55	0.44
1:A:151:THR:HG23	1:A:165:ILE:HD13	1.99	0.44
1:B:203:VAL:C	1:B:205:ARG:H	2.21	0.44
1:C:75:VAL:O	1:C:76:SER:C	2.56	0.44
1:B:225:LYS:O	1:B:228:SER:OG	2.36	0.43
1:C:140:MET:HE2	1:C:186:SER:HB3	2.00	0.43
1:B:221:GLU:H	1:B:221:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:250:ALA:C	1:D:252:ARG:H	2.22	0.43
1:C:270:ASN:HA	1:C:271:PRO:HD2	1.78	0.43
1:C:36:LYS:HG2	1:C:110:MET:HB3	2.00	0.43
1:D:276:LEU:HA	1:D:279:LEU:HD12	2.00	0.43
1:C:44:LYS:HB2	1:C:44:LYS:HE3	1.74	0.43
1:D:174:LYS:NZ	1:D:191:ASP:OD2	2.43	0.43
1:A:170:SER:O	1:A:173:GLY:N	2.37	0.43
1:A:40:THR:OG1	1:A:120:HIS:CD2	2.53	0.43
1:D:75:VAL:O	1:D:78:CYS:HB2	2.17	0.43
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.82	0.43
1:D:171:LEU:HD12	3:D:1:T30:H22	1.98	0.43
1:C:133:ILE:HD11	1:D:152:VAL:HG11	2.00	0.43
1:C:259:ASP:CG	1:C:264:THR:HG21	2.39	0.43
1:C:35:LYS:O	1:C:60:HIS:N	2.47	0.43
1:A:93:MET:HG3	1:A:120:HIS:CE1	2.54	0.43
1:A:114:ASP:O	1:A:163:GLY:CA	2.66	0.43
1:A:145:LEU:HA	1:A:145:LEU:HD12	1.90	0.42
1:D:273:ARG:HA	1:D:276:LEU:HD12	1.87	0.42
1:C:216:GLY:O	1:C:217:LEU:C	2.57	0.42
1:A:140:MET:CE	1:A:144:PHE:CD2	3.02	0.42
1:B:212:LEU:O	1:B:255:GLU:HA	2.19	0.42
1:A:215:LEU:HD11	1:A:245:ILE:HD11	2.00	0.42
1:C:50:MET:CG	1:C:242:ALA:HB1	2.49	0.42
1:C:161:SER:O	1:C:162:ASN:C	2.58	0.42
1:D:168:VAL:HG13	1:D:215:LEU:HD11	2.01	0.42
1:C:144:PHE:CD2	1:C:145:LEU:HD12	2.54	0.42
1:B:95:ASP:OD1	1:B:95:ASP:C	2.58	0.42
1:D:58:GLY:HA2	1:D:82:GLY:O	2.19	0.42
1:B:270:ASN:ND2	1:B:272:SER:H	2.17	0.42
1:B:222:THR:O	1:B:225:LYS:HB2	2.19	0.42
1:B:155:LEU:N	1:B:156:PRO:CD	2.83	0.42
1:B:158:LEU:O	1:B:159:LYS:C	2.55	0.42
1:C:219:ASP:OD2	1:C:219:ASP:O	2.38	0.42
1:B:197[B]:ILE:HG23	1:B:201:TYR:CZ	2.55	0.42
1:D:38:ILE:HG13	1:D:113:LEU:HD11	2.02	0.42
1:B:156:PRO:O	1:B:160:GLN:HG3	2.20	0.42
1:C:219:ASP:OD2	1:C:238:LYS:HG2	2.19	0.42
1:C:248:GLY:HA3	1:C:256:VAL:HG21	2.00	0.42
1:B:214:VAL:HG12	1:B:214:VAL:O	2.19	0.42
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.88	0.42
1:A:75:VAL:O	1:A:78:CYS:HB2	2.20	0.42
1:C:64:THR:HB	1:C:102:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:40:THR:HG1	1:D:120:HIS:HD2	1.64	0.42
1:B:157:MET:O	1:B:160:GLN:N	2.52	0.42
1:D:124:THR:HG21	1:D:135:HIS:HE1	1.79	0.42
3:B:1:T30:H16B	3:B:1:T30:C20	2.50	0.42
1:D:276:LEU:HD23	1:D:276:LEU:H	1.85	0.41
1:A:287:ASP:O	1:A:289:PHE:N	2.53	0.41
1:D:147:TYR:HA	1:D:150:LEU:HD12	2.02	0.41
1:A:46:ILE:HG22	1:A:50:MET:HE1	2.02	0.41
1:D:272:SER:O	1:D:276:LEU:CD2	2.53	0.41
1:D:169:SER:O	2:D:4:NAP:H6N	2.20	0.41
1:B:63:VAL:O	1:B:88:TYR:HA	2.21	0.41
1:B:118:LEU:O	1:B:168:VAL:HG23	2.19	0.41
1:A:243:LEU:HG	1:A:247:LYS:HE3	2.02	0.41
1:C:93:MET:HG3	1:C:120:HIS:NE2	2.35	0.41
1:A:53:HIS:O	1:A:57:MET:HG3	2.20	0.41
1:D:238:LYS:HG2	1:D:238:LYS:H	1.64	0.41
1:B:38:ILE:HG13	1:B:113:LEU:HD13	2.01	0.41
1:A:43:SER:HB3	1:A:65:ALA:CB	2.51	0.41
1:B:224:MET:HE1	1:B:235:ALA:CB	2.50	0.41
1:B:120:HIS:HE1	1:B:146:SER:OG	2.02	0.41
1:B:88:TYR:C	1:B:88:TYR:CD1	2.94	0.41
1:A:55:ALA:CB	1:A:83:ALA:HB2	2.51	0.41
1:D:105:GLN:HE21	1:D:109:LEU:CD2	2.33	0.41
1:B:38:ILE:HD13	1:B:102:PHE:CE2	2.55	0.41
1:C:69:GLU:O	1:C:73:LYS:CG	2.67	0.41
1:A:220:THR:O	1:A:221:GLU:C	2.59	0.41
1:A:116:LEU:CG	1:A:118:LEU:HD21	2.51	0.41
1:C:172:ALA:HB2	3:C:1:T30:H20	2.02	0.41
1:C:140:MET:HG2	1:D:140[B]:MET:CG	2.49	0.41
1:D:276:LEU:H	1:D:276:LEU:CD2	2.17	0.41
1:D:105:GLN:HE21	1:D:109:LEU:CD1	2.33	0.41
1:D:244:GLU:HG3	1:D:258:TYR:CD2	2.56	0.41
1:D:259:ASP:C	1:D:261:SER:H	2.23	0.41
1:C:259:ASP:HB3	1:C:265:THR:HG22	2.01	0.41
1:A:95:ASP:OD1	1:A:97:THR:N	2.54	0.41
1:D:50:MET:HE3	1:D:117:ILE:CG2	2.47	0.41
1:D:170:SER:OG	1:D:171:LEU:N	2.53	0.41
1:A:144:PHE:O	1:A:148:VAL:HG23	2.21	0.41
1:A:215:LEU:N	1:A:215:LEU:HD23	2.36	0.40
1:A:64:THR:O	1:A:65:ALA:HB2	2.21	0.40
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.21	0.40
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:64:THR:OG1	1:D:65:ALA:N	2.54	0.40
1:C:197:ILE:HG22	1:C:210:ILE:CD1	2.51	0.40
1:B:140:MET:HB3	1:B:140:MET:HE2	1.80	0.40
1:D:170:SER:HB2	2:D:4:NAP:H5N	2.03	0.40
1:D:69:GLU:H	1:D:69:GLU:HG2	1.63	0.40
1:C:36:LYS:O	1:C:113:LEU:HD12	2.22	0.40
1:A:268:ILE:HG22	1:A:269:ARG:N	2.37	0.40
1:D:88:TYR:C	1:D:88:TYR:CD1	2.93	0.40
1:B:224:MET:HE2	1:B:235:ALA:HB1	2.02	0.40
1:A:140:MET:HE3	1:A:144:PHE:CD2	2.56	0.40
1:A:195:SER:HB3	1:B:176:ALA:HB2	2.03	0.40
1:C:75:VAL:O	1:C:78:CYS:N	2.54	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	261/272 (96%)	229 (88%)	29 (11%)	3 (1%)	21	34
1	B	267/272 (98%)	230 (86%)	31 (12%)	6 (2%)	10	15
1	C	250/272 (92%)	217 (87%)	28 (11%)	5 (2%)	11	17
1	D	254/272 (93%)	201 (79%)	44 (17%)	9 (4%)	6	6
All	All	1032/1088 (95%)	877 (85%)	132 (13%)	23 (2%)	10	15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLU
1	D	205	ARG
1	A	234	GLN
1	A	288	ARG
1	B	45	GLY
1	B	263	TRP

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Mol	Chain	Res	Type
1	D	65	ALA
1	D	67	SER
1	D	275	ILE
1	B	65	ALA
1	B	264	THR
1	B	281	SER
1	C	65	ALA
1	C	204	SER
1	D	130	HIS
1	D	276	LEU
1	C	85	SER
1	C	202	SER
1	D	56	LYS
1	A	22	PRO
1	C	203	VAL
1	D	22	PRO
1	D	23	LEU

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	223/229 (97%)	206 (92%)	17 (8%)	19	33
1	B	226/229 (99%)	214 (95%)	12 (5%)	32	53
1	C	212/229 (93%)	199 (94%)	13 (6%)	26	44
1	D	216/229 (94%)	190 (88%)	26 (12%)	7	12
All	All	877/916 (96%)	809 (92%)	68 (8%)	18	31

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	GLU
1	A	44	LYS
1	A	70	THR
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	125	SER
1	A	130	HIS
1	A	131	ASP
1	A	202	SER
1	A	234	GLN
1	A	262	LEU
1	A	268	ILE
1	A	272	SER
1	A	275	ILE
1	A	276	LEU
1	A	281	SER
1	A	287	ASP
1	B	26	GLU
1	B	69	GLU
1	B	184	SER
1	B	203	VAL
1	B	228	SER
1	B	234	GLN
1	B	261	SER
1	B	265	THR
1	B	268	ILE
1	B	269	ARG
1	B	270	ASN
1	B	272	SER
1	C	43	SER
1	C	44	LYS
1	C	56	LYS
1	C	88	TYR
1	C	123	ASN
1	C	145	LEU
1	C	160	GLN
1	C	162	ASN
1	C	197	ILE
1	C	205	ARG
1	C	221	GLU
1	C	262	LEU
1	C	269	ARG
1	D	21	GLN
1	D	43	SER
1	D	69	GLU
1	D	76	SER
1	D	80	GLU

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Mol	Chain	Res	Type
1	D	88	TYR
1	D	92	THR
1	D	109	LEU
1	D	145	LEU
1	D	146	SER
1	D	161	SER
1	D	179	MET
1	D	205	ARG
1	D	209	SER
1	D	222	THR
1	D	225	LYS
1	D	252	ARG
1	D	261	SER
1	D	263	TRP
1	D	266	LEU
1	D	267	LEU
1	D	268	ILE
1	D	270	ASN
1	D	272	SER
1	D	275	ILE
1	D	276	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	87	HIS
1	A	119	ASN
1	A	120	HIS
1	A	127	ASN
1	A	207	ASN
1	A	270	ASN
1	B	77	HIS
1	B	119	ASN
1	B	120	HIS
1	B	160	GLN
1	B	234	GLN
1	B	253	GLN
1	B	270	ASN
1	C	72	GLN
1	C	77	HIS
1	C	119	ASN

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Mol	Chain	Res	Type
1	C	123	ASN
1	C	160	GLN
1	D	53	HIS
1	D	87	HIS
1	D	105	GLN
1	D	119	ASN
1	D	120	HIS
1	D	160	GLN
1	D	234	GLN
1	D	270	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	$\# Z > 2$
2	NAP	A	1	-	52,52,52	1.32	3 (5%)	80,80,80	1.84	11 (13%)
3	T30	A	293	-	32,32,32	1.10	3 (9%)	47,49,49	2.00	8 (17%)
3	T30	B	1	-	32,32,32	1.12	3 (9%)	47,49,49	2.19	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	2	-	52,52,52	1.33	2 (3%)	80,80,80	1.77	10 (12%)
3	T30	C	1	-	32,32,32	1.30	4 (12%)	47,49,49	2.33	8 (17%)
2	NAP	C	3	-	52,52,52	1.32	2 (3%)	80,80,80	1.84	15 (18%)
3	T30	D	1	-	32,32,32	1.30	4 (12%)	47,49,49	2.10	10 (21%)
2	NAP	D	4	-	52,52,52	1.35	3 (5%)	80,80,80	1.66	8 (10%)

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
2	NAP	A	1	-	-	0/35/67/67	0/3/5/5
3	T30	A	293	-	-	0/19/29/29	0/3/4/4
3	T30	B	1	-	-	0/19/29/29	0/3/4/4
2	NAP	B	2	-	-	0/35/67/67	0/3/5/5
3	T30	C	1	-	-	0/19/29/29	0/3/4/4
2	NAP	C	3	-	-	0/35/67/67	0/3/5/5
3	T30	D	1	-	-	0/19/29/29	0/3/4/4
2	NAP	D	4	-	-	0/35/67/67	0/3/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAP	O7N-C7N	7.29	1.41	1.24
2	C	3	NAP	O7N-C7N	7.07	1.40	1.24
2	D	4	NAP	O7N-C7N	7.04	1.40	1.24
2	A	1	NAP	O7N-C7N	7.03	1.40	1.24
3	D	1	T30	C2-N6	-3.61	1.32	1.36
3	C	1	T30	C1-C3	-3.36	1.49	1.54
3	B	1	T30	C1-C3	-3.33	1.49	1.54
2	B	2	NAP	C2A-N3A	3.22	1.38	1.32
3	D	1	T30	C1-C3	-3.21	1.49	1.54
3	C	1	T30	C2-N6	-3.18	1.33	1.36
2	D	4	NAP	C2A-N3A	3.14	1.38	1.32
3	C	1	T30	C10-N12	3.12	1.36	1.33
2	A	1	NAP	C2A-N3A	3.08	1.38	1.32
3	D	1	T30	C1-C2	-2.80	1.49	1.53
2	C	3	NAP	C2A-N3A	2.72	1.37	1.32
3	A	293	T30	C1-C3	-2.60	1.50	1.54
3	C	1	T30	C1-C2	-2.57	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	T30	C10-N12	2.41	1.36	1.33
3	D	1	T30	C10-N12	2.33	1.35	1.33
3	B	1	T30	C10-N12	2.27	1.35	1.33
3	A	293	T30	C2-N7	2.25	1.35	1.31
2	A	1	NAP	C2D-C1D	-2.23	1.50	1.53
3	B	1	T30	C2-N6	-2.21	1.34	1.36
2	D	4	NAP	C2A-N1A	2.14	1.38	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAP	N3A-C2A-N1A	-10.43	119.99	128.71
2	C	3	NAP	N3A-C2A-N1A	-10.09	120.27	128.71
3	B	1	T30	C1-C2-N6	9.99	125.86	123.67
2	A	1	NAP	N3A-C2A-N1A	-9.86	120.46	128.71
2	D	4	NAP	N3A-C2A-N1A	-9.55	120.73	128.71
3	A	293	T30	C10-N6-C2	-8.63	104.04	108.48
3	C	1	T30	C10-N6-C2	-8.46	104.13	108.48
3	C	1	T30	C1-C2-N6	-8.02	121.91	123.67
3	D	1	T30	C10-N6-C2	-7.21	104.77	108.48
2	A	1	NAP	O4D-C1D-N1N	7.00	115.12	107.95
3	C	1	T30	N7-C2-N6	6.80	115.86	111.11
3	D	1	T30	C4-C1-C3	-5.85	110.01	118.28
3	B	1	T30	C10-N6-C2	-5.83	105.48	108.48
3	A	293	T30	N7-C2-N6	5.66	115.06	111.11
3	D	1	T30	N7-C2-N6	5.57	115.00	111.11
2	B	2	NAP	O4D-C1D-N1N	4.99	113.06	107.95
2	A	1	NAP	O4B-C1B-N9A	4.91	113.01	108.44
3	B	1	T30	N7-C2-N6	4.52	114.27	111.11
2	C	3	NAP	C3N-C7N-N7N	4.18	122.53	117.77
2	C	3	NAP	O4B-C1B-C2B	-4.17	103.05	106.95
2	D	4	NAP	C3N-C7N-N7N	4.14	122.48	117.77
2	B	2	NAP	O4B-C1B-N9A	4.08	112.24	108.44
2	A	1	NAP	C2D-C1D-N1N	-4.07	106.97	113.86
3	A	293	T30	C4-C1-C3	-3.98	112.66	118.28
2	C	3	NAP	O4D-C1D-N1N	3.97	112.01	107.95
2	D	4	NAP	N3A-C4A-N9A	3.81	132.31	125.43
3	D	1	T30	C4-C1-C2	-3.70	112.17	118.87
2	B	2	NAP	N3A-C4A-N9A	3.69	132.10	125.43
2	C	3	NAP	O4B-C1B-N9A	-3.68	105.02	108.44
2	A	1	NAP	N3A-C4A-N9A	3.46	131.68	125.43
3	D	1	T30	C1-C2-N6	-3.34	122.94	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAP	N3A-C4A-N9A	3.08	130.99	125.43
3	C	1	T30	C4-C1-C5	3.05	60.59	58.63
2	D	4	NAP	O7N-C7N-C3N	-3.01	116.19	119.58
3	D	1	T30	C4-C1-C5	2.98	60.55	58.63
3	B	1	T30	C4-C1-C5	2.87	60.48	58.63
3	B	1	T30	C16-C11-N6	-2.85	108.18	111.52
3	A	293	T30	C4-C1-C2	-2.84	113.72	118.87
2	B	2	NAP	O7N-C7N-N7N	-2.75	118.61	122.59
2	C	3	NAP	O7N-C7N-N7N	-2.73	118.64	122.59
2	C	3	NAP	O4D-C1D-C2D	-2.73	102.59	106.77
2	B	2	NAP	C5A-C4A-N3A	-2.72	119.77	125.70
2	B	2	NAP	C2A-N3A-C4A	2.71	121.71	114.01
2	D	4	NAP	P2B-O2B-C2B	-2.67	116.34	121.96
2	C	3	NAP	C4A-C5A-N7A	-2.66	107.24	109.52
3	C	1	T30	C2-N7-N12	-2.66	102.09	106.06
2	A	1	NAP	C4A-C5A-N7A	-2.61	107.28	109.52
3	B	1	T30	C15-C10-N6	2.56	128.33	124.76
3	A	293	T30	C2-N7-N12	-2.54	102.27	106.06
3	D	1	T30	C2-N7-N12	-2.46	102.39	106.06
3	A	293	T30	C14-C18-C13	-2.45	119.57	122.90
3	B	1	T30	C2-N7-N12	-2.41	102.46	106.06
3	C	1	T30	C8-C3-C9	2.41	121.59	117.94
3	D	1	T30	C20-C15-C10	-2.38	116.25	120.61
2	D	4	NAP	C2D-C1D-N1N	-2.36	109.86	113.86
3	C	1	T30	C4-C1-C3	-2.33	114.98	118.28
2	A	1	NAP	C5A-C4A-N3A	-2.32	120.64	125.70
3	A	293	T30	C4-C1-C5	2.30	60.11	58.63
3	A	293	T30	C15-C10-N6	2.29	127.96	124.76
2	C	3	NAP	C2D-C1D-N1N	-2.26	110.03	113.86
2	B	2	NAP	C4A-C5A-N7A	-2.26	107.59	109.52
2	C	3	NAP	N7A-C8A-N9A	-2.23	108.06	114.36
2	A	1	NAP	C5B-C4B-C3B	-2.21	106.37	115.21
2	D	4	NAP	N7A-C8A-N9A	-2.21	108.12	114.36
2	A	1	NAP	C2A-N3A-C4A	2.20	120.28	114.01
3	D	1	T30	C17-C11-N6	-2.18	108.97	111.52
2	C	3	NAP	C2A-N3A-C4A	2.17	120.19	114.01
3	C	1	T30	C15-C10-N6	2.16	127.77	124.76
2	C	3	NAP	O5D-C5D-C4D	-2.13	101.11	108.94
2	C	3	NAP	O2A-PA-O3	2.12	115.22	105.14
2	A	1	NAP	N7A-C8A-N9A	-2.12	108.36	114.36
2	D	4	NAP	C5A-C4A-N3A	-2.10	121.13	125.70
3	D	1	T30	C8-C3-C9	2.09	121.12	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAP	O7N-C7N-N7N	-2.09	119.58	122.59
2	B	2	NAP	N7A-C8A-N9A	-2.06	108.52	114.36
3	B	1	T30	C14-C18-C13	-2.06	120.10	122.90
2	C	3	NAP	C5A-C4A-N3A	-2.05	121.24	125.70
2	B	2	NAP	C3N-C7N-N7N	2.03	120.08	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	264/272 (97%)	0.29	10 (3%) 38 41	39, 62, 94, 108	0
1	B	264/272 (97%)	0.38	13 (4%) 28 30	39, 58, 86, 101	0
1	C	253/272 (93%)	0.32	9 (3%) 41 43	37, 58, 79, 90	0
1	D	257/272 (94%)	0.68	30 (11%) 5 5	40, 77, 99, 115	0
All	All	1038/1088 (95%)	0.42	62 (5%) 22 22	37, 62, 96, 115	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	10.0
1	B	231	VAL	6.6
1	A	23	LEU	6.3
1	D	22	PRO	5.3
1	D	24	ASN	4.5
1	D	263	TRP	4.3
1	A	263	TRP	3.9
1	D	226	ALA	3.9
1	B	177	TYR	3.8
1	C	23	LEU	3.8
1	D	74	VAL	3.7
1	C	263	TRP	3.7
1	A	249	GLY	3.7
1	D	32	LEU	3.6
1	C	267	LEU	3.6
1	D	62	VAL	3.3
1	D	212	LEU	3.2
1	C	27	PHE	3.2
1	D	278	PHE	3.2
1	D	63	VAL	3.1
1	B	278	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	279	LEU	3.0
1	A	284	TYR	3.0
1	A	25	GLU	2.9
1	B	268	ILE	2.9
1	A	286	MET	2.9
1	D	79	LEU	2.9
1	D	60	HIS	2.8
1	B	263	TRP	2.8
1	B	230	ILE	2.8
1	D	38	ILE	2.7
1	C	266	LEU	2.7
1	D	21	GLN	2.7
1	C	268	ILE	2.7
1	B	23	LEU	2.6
1	D	81	LEU	2.6
1	C	175	VAL	2.6
1	B	266	LEU	2.6
1	B	267	LEU	2.6
1	D	251	LEU	2.5
1	B	21	GLN	2.5
1	D	145	LEU	2.5
1	D	218	ILE	2.4
1	D	51	ALA	2.3
1	D	160	GLN	2.3
1	B	284	TYR	2.3
1	D	87	HIS	2.3
1	B	282	THR	2.3
1	D	280	TYR	2.2
1	C	212	LEU	2.2
1	D	50	MET	2.2
1	A	21	GLN	2.2
1	D	223	ALA	2.1
1	D	113	LEU	2.1
1	A	63	VAL	2.1
1	B	197[A]	ILE	2.1
1	D	177	TYR	2.1
1	D	257	TYR	2.1
1	A	212	LEU	2.1
1	D	54	LEU	2.1
1	A	285	ASN	2.0
1	D	64	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	T30	C	1	29/29	0.29	1.79	90,92,98,99	0
3	T30	D	1	29/29	0.28	1.12	82,83,84,84	0
3	T30	A	293	29/29	0.18	0.08	63,65,66,68	0
3	T30	B	1	29/29	0.16	-0.23	62,66,68,68	0
2	NAP	B	2	48/48	0.14	-0.29	41,49,54,57	0
2	NAP	C	3	48/48	0.14	-0.39	42,47,52,54	0
2	NAP	A	1	48/48	0.14	-0.77	42,48,54,57	0
2	NAP	D	4	48/48	0.13	-0.94	60,62,70,72	0

6.5 Other polymers

There are no such residues in this entry.