



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 6CSF / pdb_00006csf
Title : Crystal structure of sodium/alanine symporter AgcS with D-alanine bound
Authors : Ma, J.; Reyes, F.E.; Gonen, T.
Deposited on : 2018-03-20
Resolution : 3.30 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

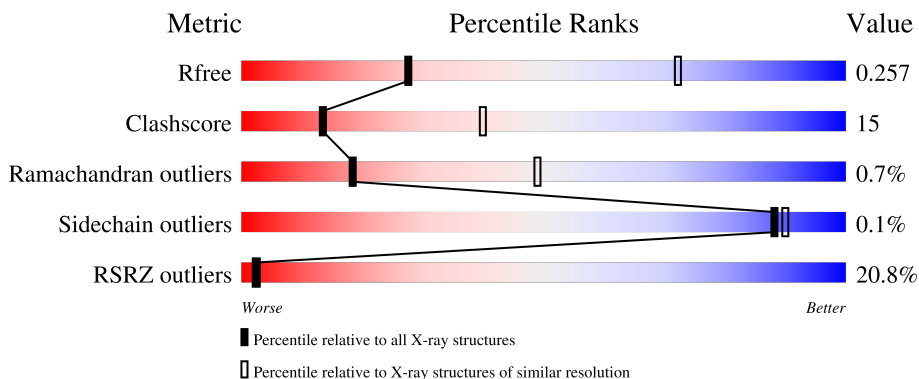
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	214	
1	H	214	
2	B	213	
2	L	213	
3	C	453	

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Mol	Chain	Length	Quality of chain
3	M	453	

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
5	DAL	M	502	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12670 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 Monoclonal antibody FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1556	973	259	315	9	0	0	0
1	H	214	1556	973	259	315	9	0	0	0

- Molecule 2 is a protein called Monoclonal antibody FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	1606	998	273	328	7	0	0	0
2	L	213	1606	998	273	328	7	0	0	0

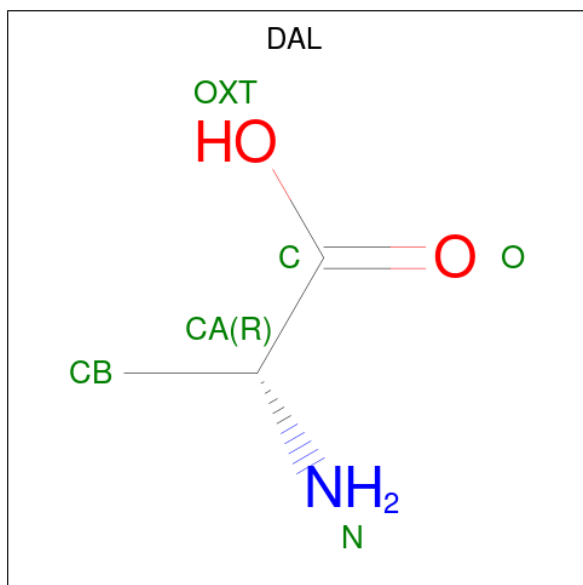
- Molecule 3 is a protein called Sodium/alanine symporter AgcS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	431	3183	2113	498	555	17	0	0	0
3	C	428	3156	2094	495	550	17	0	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Na	0	0
			1	1		

- Molecule 5 is D-ALANINE (CCD ID: DAL) (formula: C₃H₇NO₂).

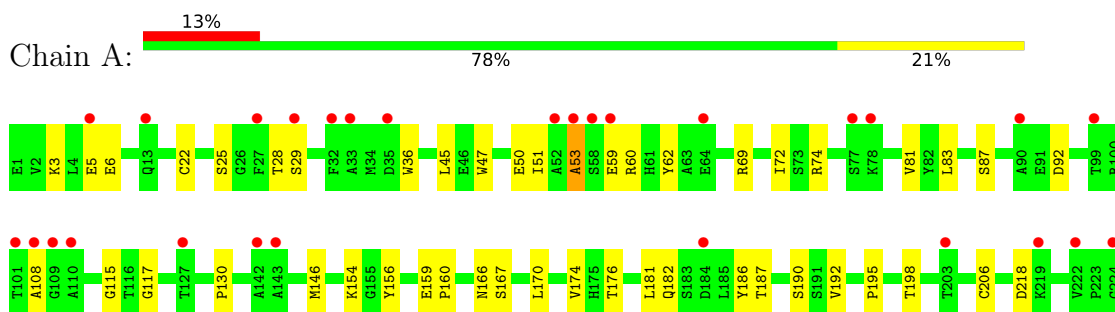


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	6	3	1	2	0	0

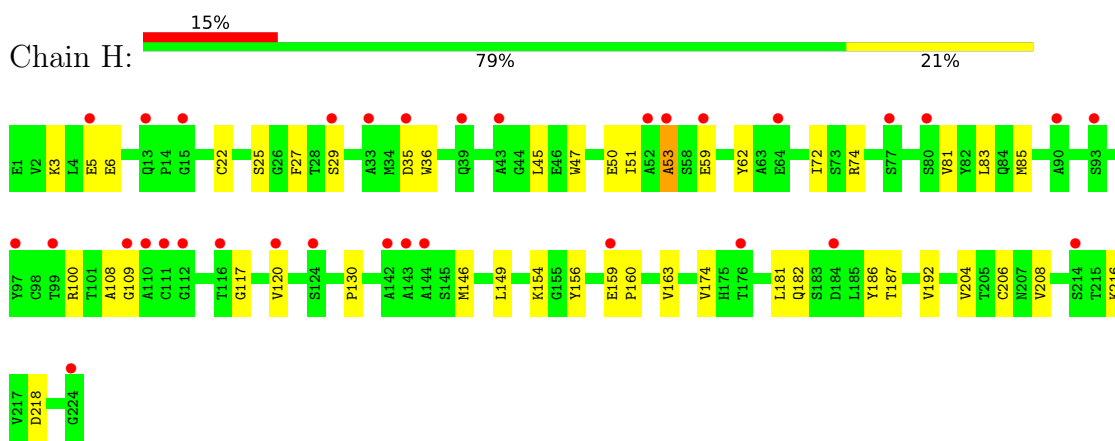
3 Residue-property plots [i](#)

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.

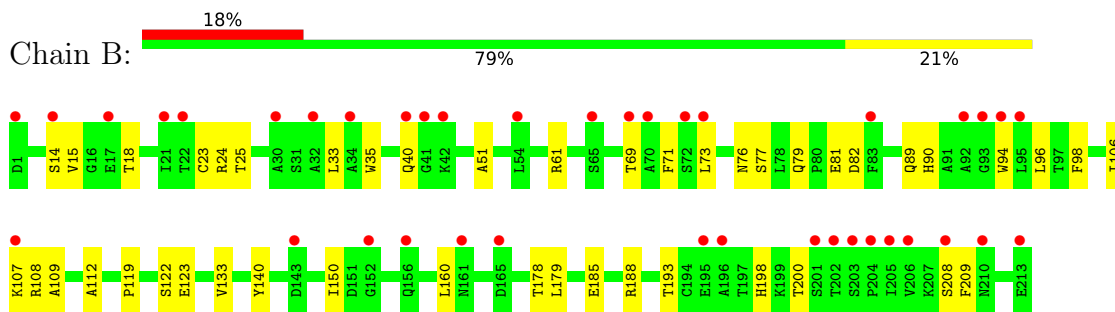
- Molecule 1: Monoclonal antibody FAB heavy chain



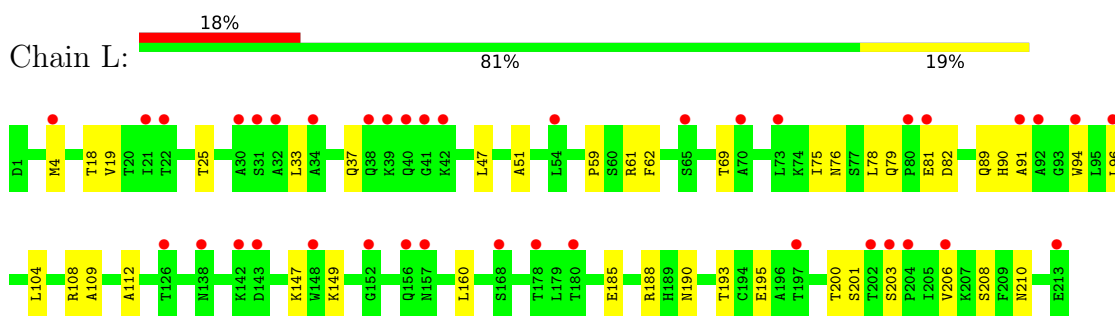
- Molecule 1: Monoclonal antibody FAB heavy chain



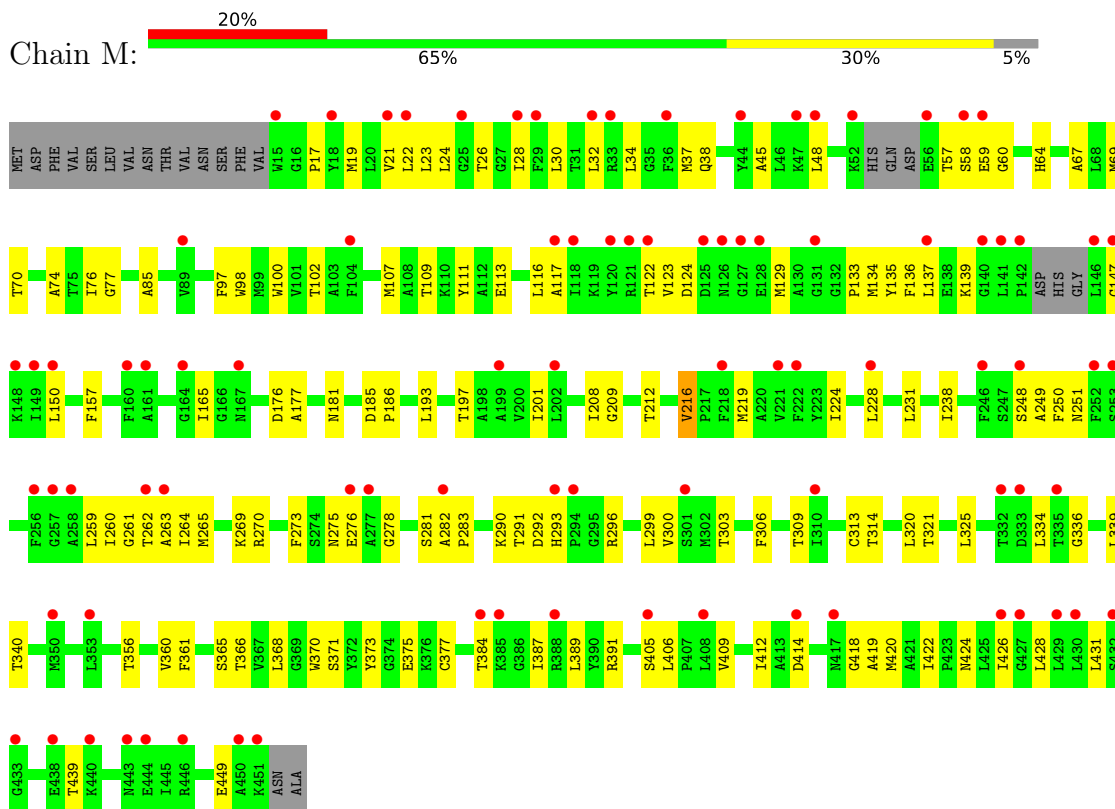
- Molecule 2: Monoclonal antibody FAB light chain



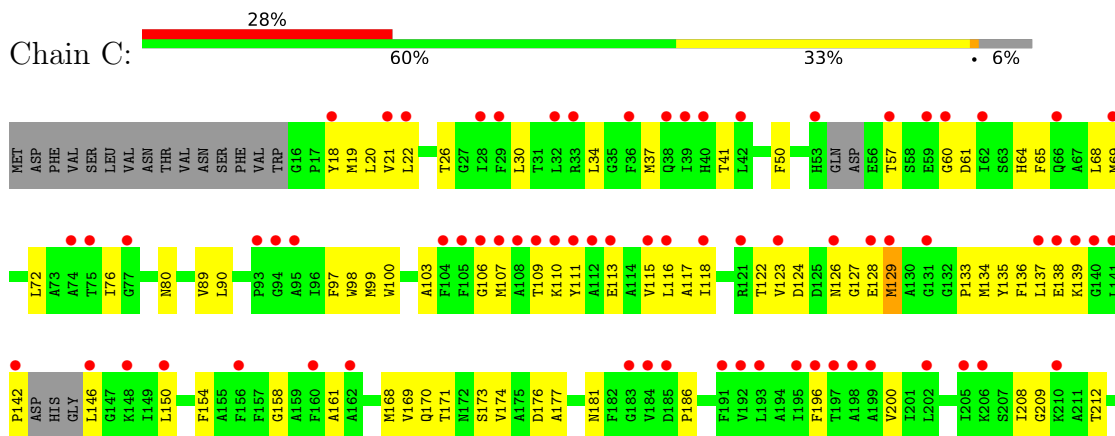
- Molecule 2: Monoclonal antibody FAB light chain

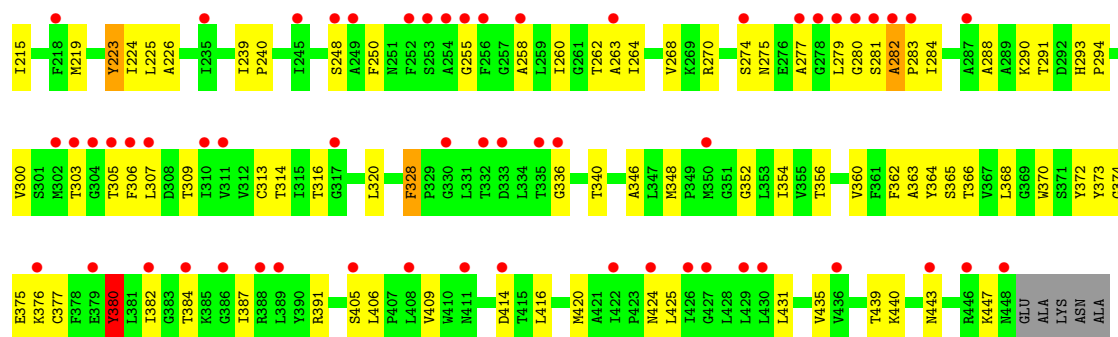


• Molecule 3: Sodium/alanine symporter AgcS



• Molecule 3: Sodium/alanine symporter AgcS





4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	183.05Å 183.05Å 349.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	158.53 – 3.30 158.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (158.53-3.30) 99.9 (158.53-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.240 , 0.253 0.242 , 0.257	Depositor DCC
R_{free} test set	4920 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	112.8	Xtrriage
Anisotropy	0.181	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 104.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/1593	0.48	0/2177
1	H	0.20	0/1593	0.48	0/2177
2	B	0.19	0/1639	0.43	0/2225
2	L	0.18	0/1639	0.45	0/2225
3	C	0.30	2/3229 (0.1%)	0.44	0/4390
3	M	0.20	1/3257 (0.0%)	0.38	0/4428
All	All	0.23	3/12950 (0.0%)	0.44	0/17622

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	216	VAL	CA-CB	-5.26	1.51	1.54
3	C	380	TYR	C-O	-5.16	1.18	1.24
3	C	223	TYR	N-CA	-5.10	1.39	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1556	0	1510	35	0
1	H	1556	0	1510	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1606	0	1554	41	0
2	L	1606	0	1554	36	0
3	C	3156	0	3246	133	0
3	M	3183	0	3272	113	0
4	M	1	0	0	0	0
5	M	6	0	6	8	0
All	All	12670	0	12652	372	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 (372) 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)
3:C:65:PHE:CE2	3:C:69:MET:HE2	1.73	1.21
3:C:284:ILE:HG21	3:C:373:TYR:HA	1.39	1.04
3:C:282:ALA:H	3:C:283:PRO:HD2	1.26	1.00
3:C:281:SER:O	3:C:373:TYR:CE2	2.20	0.95
3:C:282:ALA:H	3:C:283:PRO:CD	1.82	0.92
3:M:77:GLY:HA3	5:M:502:DAL:O	1.73	0.88
2:L:91:ALA:HA	2:L:96:LEU:CD2	2.04	0.88
2:L:90:HIS:O	2:L:96:LEU:HD23	1.74	0.86
3:C:282:ALA:N	3:C:283:PRO:HD2	1.92	0.85
3:M:165:ILE:CG2	5:M:502:DAL:HB2	2.08	0.83
3:C:281:SER:O	3:C:373:TYR:HE2	1.60	0.81
1:H:22:CYS:HB3	1:H:81:VAL:HG12	1.63	0.80
1:A:47:TRP:HZ2	1:A:50:GLU:HB2	1.51	0.76
3:M:57:THR:HA	3:M:290:LYS:HD3	1.67	0.76
2:L:90:HIS:O	2:L:96:LEU:CD2	2.33	0.75
3:M:64:HIS:HE1	3:M:296:ARG:HG2	1.50	0.75
2:L:91:ALA:HA	2:L:96:LEU:HD21	1.69	0.75
3:C:284:ILE:O	3:C:372:TYR:HE2	1.69	0.75
3:C:281:SER:O	3:C:373:TYR:CD2	2.40	0.74
2:B:24:ARG:HH11	2:B:25:THR:HG22	1.52	0.73
3:C:270:ARG:NH2	3:C:414:ASP:OD2	2.21	0.73
2:B:96:LEU:HD23	2:B:96:LEU:H	1.54	0.73
3:M:292:ASP:OD2	3:M:296:ARG:NH1	2.21	0.72
2:B:24:ARG:CZ	2:B:24:ARG:HA	2.19	0.72
3:C:69:MET:SD	3:C:69:MET:N	2.62	0.72
3:C:284:ILE:O	3:C:372:TYR:CE2	2.44	0.71
3:M:77:GLY:CA	5:M:502:DAL:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:MET:CG	3:C:380:TYR:HD2	2.04	0.71
1:A:22:CYS:HB3	1:A:81:VAL:HG12	1.71	0.70
3:C:293:HIS:CG	3:C:294:PRO:HD2	2.26	0.70
2:B:185:GLU:OE2	2:B:188:ARG:NH2	2.25	0.70
3:C:18:TYR:O	3:C:21:VAL:HG22	1.93	0.69
3:C:134:MET:CG	3:C:380:TYR:CD2	2.76	0.69
3:M:113:GLU:HB3	3:M:283:PRO:HG3	1.74	0.69
1:A:5:GLU:HB2	1:H:146:MET:HE1	1.75	0.69
3:C:118:ILE:HG12	3:C:294:PRO:HD3	1.74	0.68
3:M:60:GLY:HA2	3:M:129:MET:HE1	1.74	0.68
3:C:20:LEU:HD23	3:C:268:VAL:HG12	1.76	0.68
3:C:406:LEU:HB3	3:C:409:VAL:HB	1.75	0.68
2:B:61:ARG:NH1	2:L:79:GLN:OE1	2.26	0.68
3:C:177:ALA:O	3:C:181:ASN:ND2	2.26	0.67
3:M:116:LEU:HD21	3:M:431:LEU:HB2	1.77	0.67
3:C:137:LEU:HD13	3:C:150:LEU:HB3	1.77	0.67
3:C:134:MET:HG2	3:C:380:TYR:CD2	2.29	0.67
3:M:406:LEU:HB3	3:M:409:VAL:HB	1.76	0.67
3:M:219:MET:HE1	3:M:365:SER:HB3	1.75	0.66
3:C:65:PHE:CD2	3:C:69:MET:HE2	2.30	0.66
1:A:29:SER:O	1:A:74:ARG:NH1	2.28	0.66
3:M:281:SER:HB3	3:M:420:MET:HE1	1.78	0.66
2:L:185:GLU:OE2	2:L:188:ARG:NH2	2.28	0.66
3:C:219:MET:HE1	3:C:365:SER:HB3	1.78	0.66
3:C:127:GLY:O	3:C:129:MET:N	2.26	0.66
1:A:146:MET:HE1	1:H:5:GLU:HB2	1.78	0.66
3:M:320:LEU:HD21	3:M:340:THR:HG22	1.78	0.65
3:M:375:GLU:OE2	3:M:391:ARG:NE	2.26	0.65
1:A:174:VAL:HG12	1:A:192:VAL:HG23	1.78	0.65
3:M:292:ASP:OD1	3:M:292:ASP:N	2.31	0.64
3:C:375:GLU:OE2	3:C:391:ARG:NE	2.25	0.64
2:L:89:GLN:HE21	2:L:96:LEU:HD22	1.62	0.64
1:A:59:GLU:HB2	3:C:405:SER:HA	1.79	0.64
2:L:91:ALA:HA	2:L:96:LEU:HD23	1.80	0.61
2:B:122:SER:OG	2:B:123:GLU:OE2	2.18	0.61
3:C:65:PHE:HE2	3:C:69:MET:HE2	1.53	0.61
3:M:23:LEU:HG	3:M:278:GLY:HA3	1.83	0.61
1:H:47:TRP:HZ2	1:H:50:GLU:HB2	1.65	0.61
3:M:260:ILE:HA	3:M:264:ILE:HG12	1.83	0.61
2:B:18:THR:HG22	2:B:77:SER:H	1.66	0.60
3:M:165:ILE:HG22	5:M:502:DAL:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:109:THR:O	3:M:113:GLU:HG3	2.02	0.59
3:C:134:MET:HG3	3:C:380:TYR:HD2	1.67	0.59
2:B:193:THR:HG23	2:B:208:SER:HB3	1.84	0.59
3:C:282:ALA:N	3:C:283:PRO:CD	2.47	0.59
3:C:76:ILE:O	3:C:366:THR:OG1	2.20	0.58
3:M:19:MET:SD	3:M:418:GLY:HA2	2.43	0.58
2:L:193:THR:HG23	2:L:208:SER:HB3	1.85	0.58
1:H:174:VAL:HG12	1:H:192:VAL:HG23	1.86	0.58
2:L:108:ARG:NH1	2:L:109:ALA:O	2.37	0.58
2:B:81:GLU:HG2	2:L:81:GLU:HG3	1.85	0.58
3:M:405:SER:HA	1:H:59:GLU:HB2	1.86	0.58
2:B:24:ARG:HH22	2:B:71:PHE:H	1.50	0.58
2:L:89:GLN:NE2	2:L:96:LEU:HD22	2.19	0.58
3:C:239:ILE:HG23	3:C:240:PRO:HD3	1.86	0.57
1:A:166:ASN:HD22	1:A:170:LEU:HD13	1.68	0.57
1:H:159:GLU:HG3	1:H:160:PRO:HA	1.86	0.57
2:B:24:ARG:NH1	2:B:25:THR:HG22	2.18	0.57
3:M:70:THR:HG22	3:M:208:ILE:HG22	1.87	0.57
3:M:64:HIS:CE1	3:M:296:ARG:HG2	2.36	0.57
1:A:3:LYS:HE3	1:A:25:SER:HB2	1.86	0.57
1:A:159:GLU:HG3	1:A:160:PRO:HA	1.86	0.57
3:C:142:PRO:O	3:C:146:LEU:N	2.37	0.57
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.38	0.57
1:A:170:LEU:HD23	1:A:192:VAL:HG21	1.86	0.57
3:M:276:GLU:OE2	3:M:370:TRP:NE1	2.33	0.57
3:C:118:ILE:HB	3:C:294:PRO:HB3	1.87	0.56
2:B:40:GLN:CD	2:B:40:GLN:H	2.13	0.56
3:M:135:TYR:O	3:M:139:LYS:HG2	2.06	0.56
3:M:60:GLY:HA3	3:M:290:LYS:HA	1.87	0.56
3:M:292:ASP:OD1	3:M:296:ARG:HD2	2.05	0.56
3:C:328:PHE:CE1	3:C:346:ALA:HB1	2.41	0.56
2:L:147:LYS:HE3	2:L:149:LYS:HE3	1.88	0.56
3:M:22:LEU:O	3:M:26:THR:HG23	2.06	0.56
1:A:195:PRO:O	1:A:198:THR:OG1	2.24	0.56
3:C:262:THR:OG1	3:C:263:ALA:N	2.38	0.56
3:C:380:TYR:CD1	3:C:380:TYR:C	2.84	0.56
3:M:157:PHE:CD2	3:M:419:ALA:HB1	2.42	0.55
3:M:281:SER:HB2	3:M:373:TYR:HD2	1.71	0.55
3:C:380:TYR:HD1	3:C:380:TYR:O	1.90	0.55
3:C:122:THR:HA	3:C:129:MET:HA	1.88	0.54
3:C:196:PHE:O	3:C:364:TYR:OH	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:262:THR:OG1	3:M:263:ALA:N	2.41	0.54
3:C:223:TYR:O	3:C:224:ILE:C	2.50	0.54
2:B:112:ALA:HB2	2:B:200:THR:HG21	1.88	0.54
3:C:57:THR:HA	3:C:290:LYS:HD3	1.90	0.54
3:C:309:THR:HA	3:C:313:CYS:HB2	1.89	0.54
2:B:133:VAL:HG22	2:B:178:THR:HG23	1.90	0.53
3:M:269:LYS:NZ	3:M:414:ASP:OD2	2.35	0.53
3:M:74:ALA:HA	3:M:366:THR:HA	1.90	0.53
2:L:112:ALA:HB2	2:L:200:THR:HG21	1.89	0.53
3:M:248:SER:C	3:M:250:PHE:H	2.17	0.53
2:B:61:ARG:NH2	2:B:82:ASP:OD2	2.42	0.53
3:C:169:VAL:O	3:C:173:SER:OG	2.23	0.53
3:M:231:LEU:HB3	3:M:238:ILE:HD11	1.91	0.53
3:C:126:ASN:OD1	3:C:127:GLY:N	2.42	0.53
3:C:69:MET:O	3:C:212:THR:OG1	2.26	0.53
3:C:134:MET:HG2	3:C:380:TYR:HD2	1.66	0.53
3:C:300:VAL:O	3:C:303:THR:OG1	2.23	0.53
3:C:282:ALA:HA	3:C:373:TYR:HE2	1.74	0.53
3:M:197:THR:O	3:M:201:ILE:HG12	2.09	0.53
1:H:35:ASP:CG	1:H:47:TRP:HE1	2.17	0.53
3:C:117:ALA:HA	3:C:136:PHE:CE1	2.44	0.53
3:M:34:LEU:HD23	3:M:37:MET:SD	2.49	0.53
3:M:165:ILE:HG22	5:M:502:DAL:CB	2.39	0.53
1:H:29:SER:O	1:H:74:ARG:NH1	2.41	0.53
3:C:109:THR:O	3:C:113:GLU:HG3	2.09	0.52
3:C:380:TYR:C	3:C:380:TYR:HD1	2.18	0.52
2:B:24:ARG:HH22	2:B:71:PHE:N	2.07	0.52
2:B:24:ARG:NH2	2:B:71:PHE:H	2.08	0.52
3:C:60:GLY:HA2	3:C:129:MET:HE2	1.90	0.52
2:B:18:THR:HG22	2:B:76:ASN:HA	1.91	0.52
3:M:157:PHE:CG	3:M:419:ALA:HB1	2.45	0.52
3:C:26:THR:HG21	3:C:425:LEU:HD22	1.92	0.52
3:C:106:GLY:O	3:C:109:THR:OG1	2.20	0.52
2:B:79:GLN:OE1	2:L:61:ARG:NH1	2.41	0.52
3:M:165:ILE:HG23	3:M:273:PHE:CZ	2.45	0.52
3:M:309:THR:HA	3:M:313:CYS:HB2	1.91	0.52
3:C:65:PHE:CE2	3:C:69:MET:CE	2.69	0.52
3:C:133:PRO:HA	3:C:136:PHE:CD2	2.44	0.52
3:C:134:MET:HG3	3:C:380:TYR:CD2	2.44	0.52
3:M:270:ARG:NH2	3:M:414:ASP:OD2	2.43	0.51
3:C:111:TYR:OH	3:C:439:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.92	0.51
1:A:47:TRP:CZ2	1:A:50:GLU:HB2	2.39	0.51
2:L:78:LEU:HD21	2:L:104:LEU:HD11	1.93	0.51
3:M:69:MET:O	3:M:212:THR:OG1	2.27	0.51
3:C:113:GLU:OE1	3:C:280:GLY:HA2	2.11	0.51
1:A:130:PRO:HB3	1:A:156:TYR:HB3	1.93	0.50
2:B:24:ARG:HA	2:B:24:ARG:NH2	2.26	0.50
3:M:224:ILE:HG22	3:M:228:LEU:HD23	1.93	0.50
3:C:248:SER:C	3:C:250:PHE:H	2.19	0.50
2:L:4:MET:HE1	2:L:33:LEU:CD1	2.41	0.50
1:A:3:LYS:HB2	1:A:25:SER:HB2	1.94	0.50
3:M:97:PHE:HA	3:M:100:TRP:CE3	2.46	0.50
3:M:58:SER:OG	3:M:59:GLU:N	2.36	0.50
3:M:405:SER:HB2	1:H:59:GLU:HB2	1.94	0.50
3:M:291:THR:OG1	3:M:293:HIS:O	2.29	0.49
1:H:85:MET:HE1	1:H:120:VAL:HG21	1.94	0.49
3:C:115:VAL:HG11	3:C:435:VAL:HG23	1.94	0.49
3:C:168:MET:HA	3:C:171:THR:HG22	1.94	0.49
3:M:133:PRO:HA	3:M:136:PHE:CD2	2.47	0.49
1:A:176:THR:HG23	1:A:190:SER:HB2	1.93	0.49
3:M:134:MET:HE3	3:M:377:CYS:HA	1.95	0.49
1:H:130:PRO:HB3	1:H:156:TYR:HB3	1.95	0.49
3:C:348:MET:HE1	3:C:354:ILE:HD12	1.93	0.49
3:M:69:MET:HG3	3:M:216:VAL:HB	1.94	0.49
3:M:185:ASP:OD1	3:M:186:PRO:HD2	2.12	0.49
3:C:134:MET:HG2	3:C:380:TYR:CE2	2.48	0.49
1:A:51:ILE:HD13	1:A:74:ARG:HB2	1.93	0.49
1:H:3:LYS:HE2	1:H:25:SER:OG	2.12	0.49
3:M:111:TYR:OH	3:M:439:THR:HG22	2.13	0.49
3:C:122:THR:OG1	3:C:127:GLY:O	2.29	0.49
3:C:134:MET:HE1	3:C:284:ILE:HD11	1.94	0.49
3:C:284:ILE:CG2	3:C:373:TYR:HA	2.28	0.48
3:C:320:LEU:HD21	3:C:340:THR:HG22	1.95	0.48
1:A:36:TRP:NE1	1:A:83:LEU:HB2	2.28	0.48
1:H:159:GLU:HG3	1:H:160:PRO:CA	2.43	0.48
3:M:85:ALA:HB1	3:M:339:LEU:HD23	1.95	0.48
3:C:61:ASP:HB2	3:C:288:ALA:HB1	1.94	0.48
2:L:18:THR:HG22	2:L:76:ASN:HA	1.95	0.48
3:C:255:GLY:HA3	3:C:258:ALA:HB3	1.96	0.48
3:C:370:TRP:HA	3:C:373:TYR:HB2	1.96	0.48
3:C:352:GLY:O	3:C:356:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:435:VAL:O	3:C:439:THR:N	2.42	0.48
1:A:53:ALA:HB3	3:C:176:ASP:OD1	2.13	0.48
3:M:107:MET:CE	3:M:306:PHE:HB2	2.44	0.48
3:C:37:MET:O	3:C:41:THR:HG22	2.13	0.48
3:C:133:PRO:HG2	3:C:280:GLY:O	2.14	0.48
3:C:208:ILE:O	3:C:212:THR:HG22	2.12	0.48
1:H:36:TRP:NE1	1:H:83:LEU:HB2	2.28	0.48
3:C:138:GLU:OE2	3:C:380:TYR:OH	2.28	0.48
2:B:24:ARG:HA	2:B:24:ARG:NE	2.29	0.48
3:M:37:MET:HE1	3:M:111:TYR:CD1	2.48	0.47
3:C:223:TYR:O	3:C:225:LEU:N	2.47	0.47
2:B:23:CYS:O	2:B:24:ARG:NH2	2.47	0.47
3:M:38:GLN:HG2	3:M:107:MET:HB3	1.95	0.47
3:M:76:ILE:O	3:M:366:THR:OG1	2.32	0.47
3:M:123:VAL:HG13	3:M:124:ASP:O	2.14	0.47
1:H:36:TRP:CE2	1:H:83:LEU:HB2	2.49	0.47
3:M:176:ASP:OD1	1:H:53:ALA:HB3	2.14	0.47
3:C:200:VAL:HG11	3:C:368:LEU:HD13	1.96	0.47
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.97	0.47
2:B:14:SER:HA	2:B:107:LYS:HB2	1.95	0.47
3:C:134:MET:N	3:C:134:MET:SD	2.88	0.47
3:C:170:GLN:O	3:C:174:VAL:HG12	2.15	0.47
1:A:69:ARG:NH1	1:A:87:SER:O	2.48	0.47
3:C:100:TRP:NE1	3:C:314:THR:OG1	2.44	0.47
3:C:117:ALA:HA	3:C:136:PHE:HE1	1.79	0.47
3:M:37:MET:HE1	3:M:111:TYR:CG	2.50	0.46
3:M:321:THR:O	3:M:325:LEU:HD23	2.15	0.46
3:C:98:TRP:CE2	3:C:264:ILE:HG12	2.51	0.46
2:B:89:GLN:HG2	2:B:90:HIS:N	2.29	0.46
1:H:154:LYS:HB2	1:H:187:THR:HG23	1.96	0.46
1:H:51:ILE:HD13	1:H:74:ARG:HB3	1.98	0.46
3:C:37:MET:HE1	3:C:111:TYR:CD2	2.51	0.46
3:C:110:LYS:HD2	3:C:305:THR:HG23	1.98	0.46
3:C:64:HIS:NE2	3:C:290:LYS:O	2.48	0.46
3:M:389:LEU:HD23	3:M:389:LEU:HA	1.84	0.46
2:B:108:ARG:NH1	2:B:109:ALA:O	2.48	0.46
2:L:94:TRP:HA	2:L:94:TRP:CE3	2.50	0.46
1:A:167:SER:OG	1:H:216:LYS:NZ	2.48	0.46
3:M:30:LEU:HD12	3:M:109:THR:HA	1.98	0.46
3:M:38:GLN:HG2	3:M:107:MET:CB	2.46	0.46
3:C:161:ALA:HA	3:C:416:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HH22	1:A:92:ASP:CG	2.24	0.46
3:M:405:SER:CA	1:H:59:GLU:HB2	2.46	0.46
2:L:190:ASN:OD1	2:L:210:ASN:ND2	2.45	0.46
3:C:260:ILE:HA	3:C:264:ILE:HB	1.96	0.45
2:L:4:MET:HE1	2:L:33:LEU:HD11	1.97	0.45
2:L:4:MET:HE2	2:L:4:MET:HB3	1.74	0.45
1:A:182:GLN:OE1	2:B:160:LEU:HD21	2.16	0.45
3:M:100:TRP:NE1	3:M:314:THR:OG1	2.46	0.45
3:C:22:LEU:O	3:C:26:THR:HG23	2.15	0.45
3:C:380:TYR:CD1	3:C:380:TYR:O	2.69	0.45
3:M:26:THR:O	3:M:30:LEU:HG	2.17	0.45
3:M:424:ASN:O	3:M:428:LEU:HG	2.17	0.45
3:C:123:VAL:HG13	3:C:124:ASP:O	2.16	0.45
2:B:108:ARG:HG3	2:B:109:ALA:O	2.17	0.45
1:H:6:GLU:CD	1:H:117:GLY:H	2.24	0.45
3:M:67:ALA:O	3:M:70:THR:OG1	2.31	0.45
3:C:76:ILE:HG23	3:C:362:PHE:CD2	2.52	0.45
3:C:97:PHE:HA	3:C:100:TRP:CE3	2.52	0.45
3:C:384:THR:O	3:C:387:ILE:HG22	2.17	0.45
2:L:108:ARG:HG3	2:L:109:ALA:O	2.16	0.45
3:C:116:LEU:HD21	3:C:431:LEU:HB2	1.99	0.45
2:L:33:LEU:O	2:L:51:ALA:N	2.37	0.44
2:L:90:HIS:O	2:L:96:LEU:HD22	2.16	0.44
3:M:45:ALA:HB2	3:M:299:LEU:HB3	1.99	0.44
3:M:133:PRO:O	3:M:137:LEU:HD22	2.16	0.44
3:M:384:THR:O	3:M:387:ILE:HG22	2.16	0.44
3:M:409:VAL:O	3:M:412:ILE:HG13	2.17	0.44
3:C:72:LEU:HD11	3:C:307:LEU:HD22	2.00	0.44
3:C:291:THR:OG1	3:C:293:HIS:O	2.34	0.44
2:B:94:TRP:CE3	2:B:94:TRP:HA	2.52	0.44
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.76	0.44
3:M:449:GLU:OE2	3:M:449:GLU:N	2.51	0.44
3:C:107:MET:CE	3:C:306:PHE:HB2	2.47	0.44
3:M:334:LEU:HD13	3:M:339:LEU:HA	1.99	0.44
1:H:27:PHE:CE2	1:H:100:ARG:HD2	2.53	0.44
3:C:443:ASN:O	3:C:447:LYS:NZ	2.51	0.44
1:A:206:CYS:O	1:A:218:ASP:HA	2.18	0.44
1:H:181:LEU:HB2	1:H:186:TYR:CE1	2.52	0.44
3:C:440:LYS:HD3	3:C:440:LYS:HA	1.67	0.44
1:A:159:GLU:HG3	1:A:160:PRO:CA	2.48	0.43
2:B:79:GLN:HE22	2:L:61:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:MET:HG3	3:C:20:LEU:HD12	2.00	0.43
2:L:59:PRO:HG2	2:L:62:PHE:CD1	2.54	0.43
2:B:150:ILE:HD11	2:B:179:LEU:HD21	2.00	0.43
2:B:198:HIS:ND1	2:B:200:THR:OG1	2.48	0.43
3:M:48:LEU:HD21	3:M:296:ARG:HG3	1.99	0.43
3:M:64:HIS:HE2	3:M:291:THR:HA	1.83	0.43
3:M:102:THR:HG22	3:M:275:ASN:HD21	1.83	0.43
2:B:24:ARG:HH12	2:B:71:PHE:HD2	1.66	0.43
3:M:177:ALA:O	3:M:181:ASN:ND2	2.48	0.43
3:M:261:GLY:HA2	3:M:265:MET:HE3	2.01	0.43
3:C:158:GLY:HA2	3:C:420:MET:HE2	2.00	0.43
2:B:61:ARG:HB3	2:B:76:ASN:O	2.18	0.43
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.54	0.43
3:C:376:LYS:HA	3:C:376:LYS:HD3	1.83	0.43
2:B:89:GLN:HB2	2:B:98:PHE:CD1	2.52	0.43
3:M:137:LEU:HG	3:M:150:LEU:HB3	2.01	0.43
3:M:260:ILE:HG13	3:M:264:ILE:HD11	1.99	0.43
3:C:99:MET:HE1	3:C:313:CYS:HB3	2.01	0.43
1:A:59:GLU:HB2	3:C:405:SER:CA	2.45	0.43
2:B:33:LEU:O	2:B:51:ALA:N	2.40	0.43
3:M:60:GLY:HA2	3:M:129:MET:CE	2.45	0.43
3:M:117:ALA:HA	3:M:136:PHE:HE1	1.83	0.43
1:H:206:CYS:O	1:H:218:ASP:HA	2.17	0.43
3:C:284:ILE:HG22	3:C:372:TYR:CE2	2.54	0.43
1:A:154:LYS:HE3	1:A:154:LYS:HB2	1.84	0.42
1:A:181:LEU:HB2	1:A:186:TYR:CE1	2.53	0.42
3:M:38:GLN:HB3	3:M:107:MET:SD	2.59	0.42
2:L:89:GLN:HG2	2:L:90:HIS:N	2.35	0.42
1:A:154:LYS:HB2	1:A:187:THR:HG23	2.00	0.42
2:L:201:SER:OG	2:L:203:SER:O	2.25	0.42
2:B:123:GLU:OE2	2:B:123:GLU:N	2.52	0.42
3:M:28:ILE:O	3:M:32:LEU:HG	2.19	0.42
3:M:136:PHE:N	3:M:136:PHE:CD1	2.88	0.42
3:M:193:LEU:HD23	3:M:193:LEU:HA	1.82	0.42
3:M:422:ILE:O	3:M:426:ILE:HG13	2.19	0.42
3:C:127:GLY:C	3:C:129:MET:H	2.23	0.42
1:A:28:THR:O	1:A:28:THR:OG1	2.34	0.42
3:M:17:PRO:O	3:M:21:VAL:HG23	2.20	0.42
3:C:37:MET:HE2	3:C:37:MET:HB3	1.80	0.42
3:C:89:VAL:HG12	3:C:90:LEU:HD12	2.02	0.42
3:C:281:SER:OG	3:C:370:TRP:CH2	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:98:TRP:NE1	3:M:249:ALA:HB1	2.34	0.42
3:M:282:ALA:N	3:M:283:PRO:HD2	2.34	0.42
3:M:300:VAL:O	3:M:303:THR:OG1	2.34	0.42
1:H:109:GLY:O	2:L:91:ALA:HB2	2.20	0.42
3:C:30:LEU:O	3:C:34:LEU:HB2	2.19	0.42
3:C:34:LEU:HD21	3:C:439:THR:HG21	2.01	0.42
3:C:103:ALA:HB2	3:C:275:ASN:HD22	1.84	0.42
3:M:117:ALA:HA	3:M:136:PHE:CE1	2.55	0.42
3:M:137:LEU:O	3:M:147:GLY:HA3	2.20	0.42
3:M:165:ILE:HD12	3:M:370:TRP:CZ2	2.54	0.42
3:C:80:ASN:ND2	3:C:274:SER:OG	2.53	0.42
3:C:136:PHE:N	3:C:136:PHE:CD1	2.86	0.42
3:C:328:PHE:CZ	3:C:346:ALA:HB1	2.55	0.42
2:L:25:THR:HG22	2:L:69:THR:HA	2.02	0.42
1:A:6:GLU:OE2	1:A:115:GLY:HA3	2.20	0.42
1:H:45:LEU:HD23	1:H:45:LEU:HA	1.77	0.42
1:H:163:VAL:HG22	1:H:208:VAL:HG22	2.02	0.42
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.02	0.42
3:M:133:PRO:HA	3:M:136:PHE:CG	2.55	0.41
3:M:368:LEU:O	3:M:371:SER:HB3	2.20	0.41
2:B:108:ARG:HG2	2:B:140:TYR:CG	2.55	0.41
3:M:122:THR:HA	3:M:129:MET:HA	2.01	0.41
3:M:356:THR:O	3:M:360:VAL:HG23	2.20	0.41
1:H:182:GLN:OE1	2:L:160:LEU:HD21	2.19	0.41
3:C:215:ILE:HG22	3:C:219:MET:HE3	2.01	0.41
3:M:181:ASN:CG	3:M:356:THR:HG21	2.44	0.41
1:H:149:LEU:HD12	1:H:204:VAL:HG11	2.01	0.41
3:C:209:GLY:HA2	3:C:212:THR:HG22	2.02	0.41
3:M:209:GLY:HA2	3:M:212:THR:HG22	2.02	0.41
3:M:165:ILE:CG2	5:M:502:DAL:CB	2.89	0.41
3:C:356:THR:O	3:C:360:VAL:HG23	2.20	0.41
3:M:219:MET:HE2	3:M:361:PHE:HB3	2.01	0.41
3:C:382:ILE:HD12	3:C:382:ILE:HA	1.94	0.41
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.56	0.41
3:C:223:TYR:OH	3:C:316:THR:OG1	2.24	0.41
3:C:68:LEU:HD13	3:C:300:VAL:O	2.21	0.41
1:A:6:GLU:CD	1:A:117:GLY:H	2.27	0.41
1:A:60:ARG:HG3	1:A:62:TYR:HE1	1.85	0.41
3:M:97:PHE:O	3:M:100:TRP:HB2	2.21	0.41
3:C:133:PRO:HB3	3:C:424:ASN:HD22	1.86	0.41
3:C:223:TYR:O	3:C:226:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:GLY:HA2	3:C:377:CYS:SG	2.61	0.41
3:M:24:LEU:O	3:M:28:ILE:HG22	2.20	0.41
3:C:239:ILE:HG23	3:C:240:PRO:CD	2.51	0.41
2:B:15:VAL:HG22	2:B:106:ILE:HG23	2.04	0.40
2:B:24:ARG:CZ	2:B:69:THR:C	2.94	0.40
3:M:251:ASN:O	3:M:259:LEU:HD23	2.21	0.40
3:M:273:PHE:CE2	5:M:502:DAL:HB1	2.56	0.40
3:M:98:TRP:CE2	3:M:264:ILE:HG22	2.57	0.40
3:C:50:PHE:CE1	3:C:69:MET:HE1	2.56	0.40
3:M:165:ILE:HG21	5:M:502:DAL:HB2	1.96	0.40
3:C:154:PHE:HZ	3:C:280:GLY:O	2.04	0.40
3:C:170:GLN:HB3	3:C:363:ALA:HB1	2.04	0.40
1:A:62:TYR:OH	1:A:72:ILE:HG22	2.22	0.40
3:M:60:GLY:HA2	3:M:129:MET:SD	2.61	0.40
3:M:281:SER:HB2	3:M:373:TYR:CD2	2.55	0.40
1:H:62:TYR:OH	1:H:72:ILE:HG22	2.21	0.40
3:C:135:TYR:O	3:C:139:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	14	43
1	H	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	14	43
2	B	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
2	L	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	C	422/453 (93%)	386 (92%)	29 (7%)	7 (2%)	7	30
3	M	425/453 (94%)	402 (95%)	22 (5%)	1 (0%)	43	71
All	All	1693/1760 (96%)	1598 (94%)	83 (5%)	12 (1%)	18	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	53	ALA
3	C	186	PRO
1	A	53	ALA
1	A	108	ALA
1	H	108	ALA
3	C	128	GLU
3	C	129	MET
3	C	277	ALA
3	C	328	PHE
3	M	336	GLY
3	C	282	ALA
3	C	336	GLY

5.3.2 Protein sidechains [i](#)

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	172/172 (100%)	172 (100%)	0	100	100
1	H	172/172 (100%)	172 (100%)	0	100	100
2	B	179/179 (100%)	179 (100%)	0	100	100
2	L	179/179 (100%)	179 (100%)	0	100	100
3	C	315/337 (94%)	313 (99%)	2 (1%)	78	81
3	M	317/337 (94%)	317 (100%)	0	100	100
All	All	1334/1376 (97%)	1332 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	279	LEU
3	C	380	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	234	ASN
3	M	293	HIS
1	H	84	GLN
3	C	424	ASN
2	L	161	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
5	DAL	M	502	-	5,5,5	1.86	1 (20%)	6,6,6	0.80	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
5	DAL	M	502	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	502	DAL	CA-C	-3.55	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	502	DAL	O-C-CA-N
5	M	502	DAL	OXT-C-CA-N
5	M	502	DAL	O-C-CA-CB
5	M	502	DAL	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	502	DAL	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.80	28 (13%) 7 6	68, 91, 123, 177	0
1	H	214/214 (100%)	0.92	33 (15%) 5 4	68, 93, 128, 155	0
2	B	213/213 (100%)	0.90	39 (18%) 3 3	71, 96, 128, 165	0
2	L	213/213 (100%)	0.98	39 (18%) 3 3	70, 96, 127, 162	0
3	C	428/453 (94%)	1.43	128 (29%) 1 1	91, 142, 194, 245	0
3	M	431/453 (95%)	1.01	89 (20%) 2 2	86, 127, 173, 210	0
All	All	1713/1760 (97%)	1.06	356 (20%) 2 2	68, 113, 172, 245	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	40	GLN	12.0
3	M	18	TYR	11.1
1	A	109	GLY	9.1
3	C	131	GLY	8.3
1	H	224	GLY	7.5
3	C	18	TYR	7.5
2	B	40	GLN	7.5
1	H	13	GLN	7.4
3	M	388	ARG	7.3
1	A	77	SER	7.2
3	M	32	LEU	7.1
3	C	184	VAL	7.1
1	H	109	GLY	7.1
1	A	224	GLY	6.8
3	M	335	THR	6.6
3	M	21	VAL	6.5
3	M	332	THR	6.3
2	B	203	SER	6.3
3	M	29	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
3	C	253	SER	6.2
3	M	430	LEU	6.2
3	C	39	ILE	6.1
3	C	21	VAL	6.1
1	H	214	SER	6.0
3	C	306	PHE	5.9
3	C	109	THR	5.7
2	B	204	PRO	5.5
1	A	101	THR	5.5
2	B	206	VAL	5.5
1	A	52	ALA	5.5
2	L	203	SER	5.5
3	M	118	ILE	5.5
3	C	335	THR	5.4
2	B	152	GLY	5.4
3	M	125	ASP	5.3
3	C	36	PHE	5.3
1	H	52	ALA	5.3
3	M	15	TRP	5.2
1	H	112	GLY	5.1
1	H	184	ASP	5.1
2	L	70	ALA	5.1
3	M	408	LEU	5.0
3	C	104	PHE	5.0
3	C	430	LEU	4.9
3	C	280	GLY	4.9
1	H	59	GLU	4.9
1	A	142	ALA	4.9
3	C	185	ASP	4.9
3	C	142	PRO	4.8
3	M	429	LEU	4.8
3	M	52	LYS	4.8
3	M	122	THR	4.8
3	C	256	PHE	4.7
2	L	31	SER	4.7
3	M	28	ILE	4.7
3	C	108	ALA	4.7
3	C	93	PRO	4.7
3	C	128	GLU	4.7
3	M	146	LEU	4.6
3	C	107	MET	4.6
3	M	121	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
3	M	433	GLY	4.6
2	L	126	THR	4.6
2	L	41	GLY	4.5
1	A	53	ALA	4.5
3	C	206	LYS	4.5
1	A	203	THR	4.5
2	B	202	THR	4.4
3	M	263	ALA	4.3
3	C	113	GLU	4.3
3	C	278	GLY	4.3
3	M	25	GLY	4.3
3	C	57	THR	4.2
2	L	34	ALA	4.2
3	M	142	PRO	4.2
3	C	310	ILE	4.2
3	C	59	GLU	4.2
1	H	53	ALA	4.1
3	M	127	GLY	4.1
3	C	75	THR	4.1
1	A	33	ALA	4.1
1	H	43	ALA	4.1
3	C	118	ILE	4.1
3	C	427	GLY	4.1
3	C	138	GLU	4.0
1	H	33	ALA	4.0
3	C	156	PHE	4.0
3	M	202	LEU	4.0
3	C	140	GLY	4.0
3	C	304	GLY	4.0
3	C	42	LEU	4.0
1	A	110	ALA	4.0
3	C	281	SER	4.0
3	M	148	LYS	3.9
1	H	110	ALA	3.9
2	L	204	PRO	3.9
3	M	294	PRO	3.9
3	C	376	LYS	3.8
3	C	121	ARG	3.8
3	C	263	ALA	3.8
3	C	389	LEU	3.7
1	H	176	THR	3.7
2	B	30	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	206	VAL	3.7
3	C	330	GLY	3.7
3	C	94	GLY	3.7
2	B	92	ALA	3.7
3	C	424	ASN	3.7
3	M	131	GLY	3.6
1	A	59	GLU	3.6
3	C	333	ASP	3.6
2	B	34	ALA	3.6
3	C	282	ALA	3.6
2	B	195	GLU	3.6
3	M	451	LYS	3.6
1	A	29	SER	3.6
3	M	140	GLY	3.5
3	C	302	MET	3.5
3	C	123	VAL	3.5
2	B	94	TRP	3.5
2	L	202	THR	3.5
3	C	33	ARG	3.5
3	M	256	PHE	3.5
2	B	69	THR	3.5
3	C	422	ILE	3.4
1	A	184	ASP	3.4
3	C	148	LYS	3.4
3	C	95	ALA	3.4
3	C	146	LEU	3.4
1	A	108	ALA	3.4
3	C	305	THR	3.4
3	M	432	SER	3.4
3	C	137	LEU	3.4
2	B	32	ALA	3.4
3	M	47	LYS	3.4
3	M	426	ILE	3.3
3	C	77	GLY	3.3
3	C	332	THR	3.3
3	M	137	LEU	3.3
2	L	94	TRP	3.3
1	H	5	GLU	3.3
2	B	65	SER	3.3
2	L	32	ALA	3.3
1	A	78	LYS	3.3
3	M	126	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	14	SER	3.3
3	M	33	ARG	3.3
3	C	317	GLY	3.3
3	C	202	LEU	3.2
3	C	139	LYS	3.2
3	C	196	PHE	3.2
3	M	161	ALA	3.2
2	B	213	GLU	3.2
3	C	283	PRO	3.2
3	M	301	SER	3.2
1	H	90	ALA	3.2
3	M	444	GLU	3.2
3	C	192	VAL	3.2
3	C	446	ARG	3.2
3	C	311	VAL	3.2
3	C	141	LEU	3.1
3	C	116	LEU	3.1
3	C	197	THR	3.1
3	M	58	SER	3.1
3	C	110	LYS	3.1
2	B	156	GLN	3.1
2	B	54	LEU	3.1
3	M	120	TYR	3.1
3	C	129	MET	3.1
1	H	29	SER	3.1
3	M	246	PHE	3.1
3	C	160	PHE	3.1
3	C	205	ILE	3.1
3	C	426	ILE	3.1
2	B	143	ASP	3.0
3	C	414	ASP	3.0
3	M	141	LEU	3.0
3	M	257	GLY	3.0
3	C	303	THR	3.0
3	M	438	GLU	3.0
2	B	208	SER	3.0
3	C	350	MET	3.0
2	L	65	SER	3.0
1	H	97	TYR	3.0
3	C	199	ALA	3.0
3	M	350	MET	3.0
3	M	248	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	96	LEU	2.9
3	C	429	LEU	2.9
3	C	111	TYR	2.9
3	M	353	LEU	2.9
3	C	32	LEU	2.9
2	B	42	LYS	2.9
3	C	60	GLY	2.9
1	H	35	ASP	2.9
1	A	5	GLU	2.9
1	A	32	PHE	2.9
2	B	205	ILE	2.9
2	B	1	ASP	2.9
3	C	249	ALA	2.9
3	M	427	GLY	2.9
3	C	386	GLY	2.9
3	C	38	GLN	2.8
3	M	36	PHE	2.8
3	C	28	ILE	2.8
2	B	22	THR	2.8
3	M	218	PHE	2.8
3	M	277	ALA	2.7
3	C	277	ALA	2.7
2	L	157	ASN	2.7
1	H	77	SER	2.7
3	C	336	GLY	2.7
3	C	411	ASN	2.7
3	M	22	LEU	2.7
3	C	195	ILE	2.7
3	C	252	PHE	2.7
3	M	221	VAL	2.7
3	M	262	THR	2.7
1	H	142	ALA	2.7
3	C	191	PHE	2.6
2	L	42	LYS	2.6
2	L	213	GLU	2.6
1	H	124	SER	2.6
2	L	92	ALA	2.6
3	C	53	HIS	2.6
3	M	56	GLU	2.6
1	A	222	VAL	2.6
3	M	228	LEU	2.6
2	B	161	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	183	GLY	2.6
3	M	117	ALA	2.6
3	M	384	THR	2.6
3	C	198	ALA	2.6
3	C	245	ILE	2.6
2	L	38	GLN	2.6
2	B	17	GLU	2.6
2	B	72	SER	2.6
2	B	73	LEU	2.6
3	C	307	LEU	2.6
3	C	379	GLU	2.6
3	C	279	LEU	2.5
2	B	210	ASN	2.5
3	C	115	VAL	2.5
2	B	196	ALA	2.5
3	M	199	ALA	2.5
3	C	62	ILE	2.5
1	A	13	GLN	2.5
3	C	388	ARG	2.5
1	A	143	ALA	2.5
3	C	29	PHE	2.5
3	M	446	ARG	2.5
1	H	80	SER	2.5
1	A	90	ALA	2.5
3	M	167	ASN	2.5
1	H	116	THR	2.5
2	L	30	ALA	2.5
2	L	156	GLN	2.5
1	H	39	GLN	2.4
1	H	143	ALA	2.4
2	L	168	SER	2.4
2	B	95	LEU	2.4
3	C	448	ASN	2.4
1	H	120	VAL	2.4
3	C	106	GLY	2.4
3	M	253	SER	2.4
2	B	165	ASP	2.4
2	B	70	ALA	2.4
3	C	254	ALA	2.4
3	C	126	ASN	2.4
3	M	258	ALA	2.4
3	M	252	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	248	SER	2.4
1	H	15	GLY	2.3
2	B	107	LYS	2.3
3	M	282	ALA	2.3
2	L	143	ASP	2.3
3	C	162	ALA	2.3
1	A	27	PHE	2.3
3	C	105	PHE	2.3
3	M	128	GLU	2.3
1	H	93	SER	2.3
3	C	69	MET	2.3
3	M	417	ASN	2.3
2	L	142	LYS	2.3
3	M	440	LYS	2.3
3	M	149	ILE	2.3
3	M	310	ILE	2.3
3	M	405	SER	2.3
3	C	40	HIS	2.3
3	C	218	PHE	2.3
3	C	382	ILE	2.3
1	H	99	THR	2.3
2	B	201	SER	2.3
3	M	385	LYS	2.3
3	C	22	LEU	2.2
3	C	405	SER	2.2
2	B	93	GLY	2.2
3	M	150	LEU	2.2
3	C	408	LEU	2.2
1	A	127	THR	2.2
2	L	180	THR	2.2
3	C	384	THR	2.2
3	M	89	VAL	2.2
3	C	66	GLN	2.2
1	A	64	GLU	2.2
3	M	414	ASP	2.2
2	B	41	GLY	2.2
2	L	81	GLU	2.2
1	H	144	ALA	2.2
1	A	35	ASP	2.2
2	L	21	ILE	2.2
2	L	39	LYS	2.2
2	L	138	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	112	ALA	2.2
1	A	58	SER	2.1
1	A	219	LYS	2.1
2	L	148	TRP	2.1
3	C	150	LEU	2.1
2	L	4	MET	2.1
1	H	64	GLU	2.1
3	M	59	GLU	2.1
3	M	164	GLY	2.1
3	C	255	GLY	2.1
3	M	160	PHE	2.1
3	M	333	ASP	2.1
2	L	178	THR	2.1
3	M	276	GLU	2.1
3	M	104	PHE	2.1
3	M	443	ASN	2.1
3	C	443	ASN	2.1
2	B	21	ILE	2.1
3	M	293	HIS	2.1
3	C	74	ALA	2.1
2	L	80	PRO	2.1
3	C	436	VAL	2.1
2	L	73	LEU	2.1
3	M	48	LEU	2.1
1	H	111	CYS	2.1
2	L	91	ALA	2.1
3	C	258	ALA	2.1
2	L	152	GLY	2.1
1	H	159	GLU	2.1
3	C	193	LEU	2.0
1	A	99	THR	2.0
2	B	83	PHE	2.0
3	M	222	PHE	2.0
2	L	54	LEU	2.0
3	C	274	SER	2.0
2	L	22	THR	2.0
2	L	197	THR	2.0
3	M	450	ALA	2.0
3	C	287	ALA	2.0
3	M	44	TYR	2.0
3	M	147	GLY	2.0
3	C	210	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	235	ILE	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(Å ²)	Q<0.9
5	DAL	M	502	6/6	0.89	0.17	126,128,135,137	0
4	NA	M	501	1/1	0.98	0.05	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.