



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:57 pm BST

PDB ID : 3WRD  
Title : Crystal Structure of the KIF5C Motor Domain Without Any Nucleotide  
Authors : Inoue, S.; Nitta, R.; Hirokawa, N.  
Deposited on : 2014-02-21  
Resolution : 2.86 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

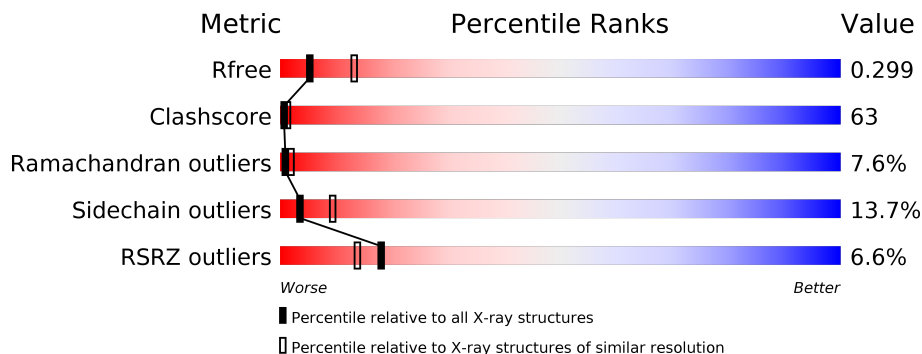
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	341	 7% 30% 48% 12% • 9%
1	B	341	 5% 39% 43% 11% • 5%

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
2	SO4	B	401	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4995 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 Kinesin heavy chain isoform 5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2436	1531	422	468	15	0	0	0
1	B	324	2544	1595	446	488	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	EXPRESSION TAG	UNP P28738
A	336	HIS	-	EXPRESSION TAG	UNP P28738
A	337	HIS	-	EXPRESSION TAG	UNP P28738
A	338	HIS	-	EXPRESSION TAG	UNP P28738
A	339	HIS	-	EXPRESSION TAG	UNP P28738
A	340	HIS	-	EXPRESSION TAG	UNP P28738
A	341	HIS	-	EXPRESSION TAG	UNP P28738
B	335	HIS	-	EXPRESSION TAG	UNP P28738
B	336	HIS	-	EXPRESSION TAG	UNP P28738
B	337	HIS	-	EXPRESSION TAG	UNP P28738
B	338	HIS	-	EXPRESSION TAG	UNP P28738
B	339	HIS	-	EXPRESSION TAG	UNP P28738
B	340	HIS	-	EXPRESSION TAG	UNP P28738
B	341	HIS	-	EXPRESSION TAG	UNP P28738

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

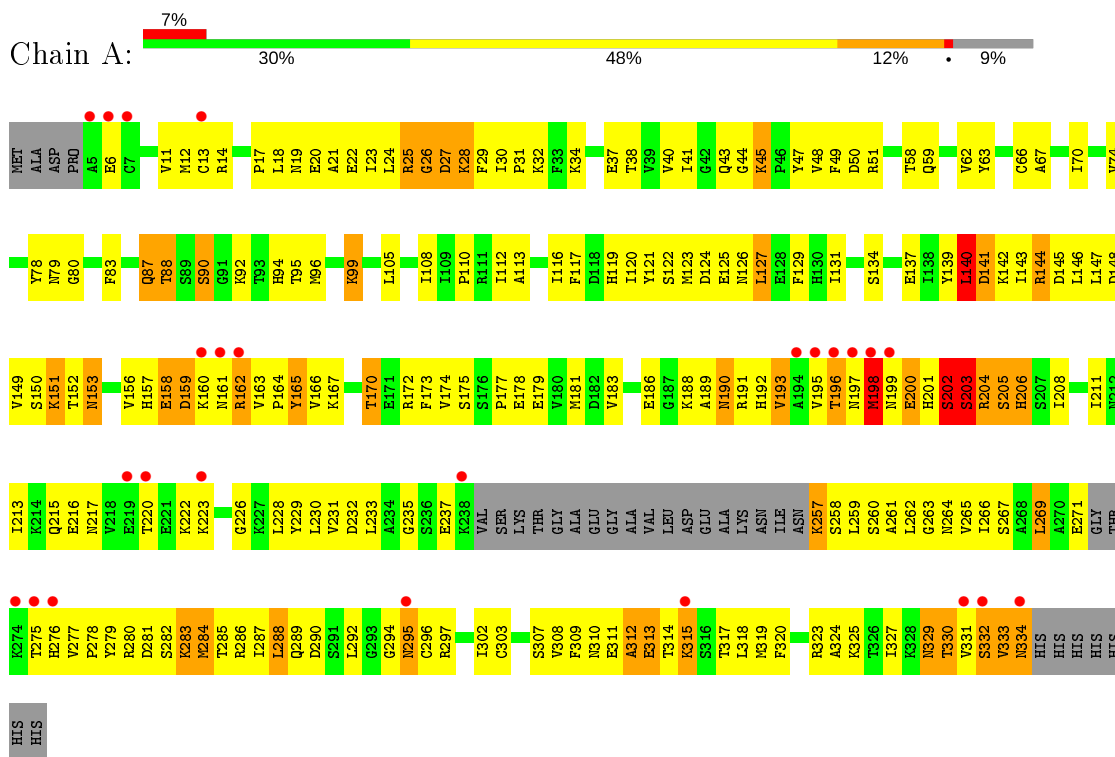
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	2	Total	O	0	0
			2	2		

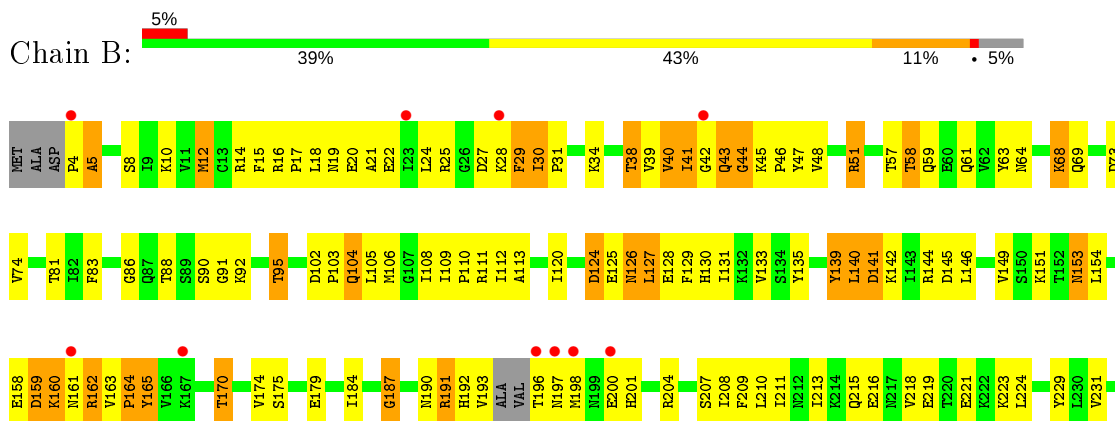
### 3 Residue-property plots [i](#)

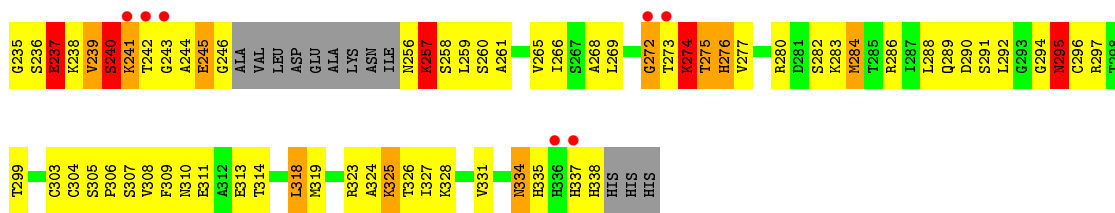
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Kinesin heavy chain isoform 5C



- Molecule 1: Kinesin heavy chain isoform 5C





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.58Å 71.32Å 176.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.86 19.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.86) 99.7 (19.83-2.86)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.88Å)	Xtrriage
Refinement program	REFMAC refmac_5.7.0032	Depositor
R, $R_{free}$	0.237 , 0.299 0.236 , 0.299	Depositor DCC
$R_{free}$ test set	1095 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.4	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 79.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4

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	0.57	0/2475	0.77	0/3334
1	B	0.65	0/2588	0.85	0/3486
All	All	0.61	0/5063	0.81	0/6820

There are no bond length outliers.

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	2436	0	2443	383	0
1	B	2544	0	2541	265	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	3	0	0	1	0
3	B	2	0	0	0	0
All	All	4995	0	4984	631	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 63.

All (631) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:CE	1:A:319:MET:HG2	1.41	1.50
1:B:193:VAL:HG21	1:B:196:THR:N	1.14	1.41
1:A:266:ILE:HG13	1:A:327:ILE:CD1	1.54	1.34
1:B:193:VAL:CG2	1:B:196:THR:N	1.88	1.32
1:A:266:ILE:CG1	1:A:327:ILE:HD11	1.60	1.30
1:A:145:ASP:OD2	1:A:170:THR:HG23	1.08	1.26
1:B:42:GLY:HA3	1:B:43:GLN:CB	1.57	1.25
1:A:296:CYS:N	1:A:331:VAL:HG12	1.50	1.25
1:A:315:LYS:CE	1:A:319:MET:CG	2.21	1.18
1:A:145:ASP:OD2	1:A:170:THR:CG2	1.91	1.18
1:B:73:ASP:OD2	1:B:297:ARG:NH1	1.78	1.17
1:A:149:VAL:HG12	1:B:319:MET:CE	1.74	1.15
1:A:315:LYS:HE2	1:A:319:MET:CG	1.76	1.15
1:B:30:ILE:HD11	1:B:308:VAL:HB	1.15	1.15
1:A:149:VAL:HG12	1:B:319:MET:HE3	1.15	1.14
1:A:174:VAL:HA	1:A:179:GLU:OE1	1.47	1.14
1:A:157:HIS:O	1:A:164:PRO:HA	1.47	1.13
1:B:30:ILE:CD1	1:B:308:VAL:HB	1.78	1.12
1:A:14:ARG:HH11	1:A:95:THR:HG22	1.10	1.12
1:A:314:THR:O	1:A:318:LEU:HD23	1.47	1.10
1:A:143:ILE:HG22	1:A:144:ARG:H	1.09	1.10
1:B:58:THR:OG1	1:B:61:GLN:HG3	1.50	1.10
1:A:315:LYS:HE3	1:A:319:MET:HG2	1.22	1.07
1:A:315:LYS:HE2	1:A:319:MET:HG2	1.17	1.07
1:B:30:ILE:HD11	1:B:308:VAL:CB	1.85	1.07
1:B:127:LEU:HD12	1:B:127:LEU:O	1.54	1.06
1:A:315:LYS:NZ	1:A:319:MET:SD	2.29	1.06
1:A:14:ARG:NH1	1:A:95:THR:HG22	1.69	1.06
1:B:159:ASP:OD1	1:B:165:TYR:CE1	2.09	1.05
1:A:29:PHE:CD1	1:A:31:PRO:HD2	1.91	1.05
1:B:42:GLY:CA	1:B:43:GLN:HB3	1.86	1.04
1:B:42:GLY:HA3	1:B:43:GLN:HB3	1.10	1.04
1:B:103:PRO:O	1:B:104:GLN:NE2	1.92	1.03
1:A:283:LYS:HG2	1:A:284:MET:H	1.24	1.02
1:B:25:ARG:HD2	1:B:27:ASP:OD1	1.60	1.02
1:B:41:ILE:N	1:B:41:ILE:HD13	1.71	1.01
1:A:196:THR:H	1:A:197:ASN:HA	1.26	0.99
1:B:274:LYS:NZ	1:B:274:LYS:O	1.94	0.99
1:A:28:LYS:O	1:A:28:LYS:NZ	1.95	0.99
1:B:30:ILE:HB	1:B:31:PRO:HD3	1.44	0.98
1:A:143:ILE:HG22	1:A:144:ARG:N	1.72	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG13	1:A:327:ILE:HD11	1.01	0.98
1:B:245:GLU:HG3	1:B:246:GLY:H	1.29	0.98
1:A:156:VAL:O	1:A:157:HIS:ND1	1.97	0.96
1:B:274:LYS:O	1:B:275:THR:HG23	1.67	0.95
1:A:143:ILE:CG2	1:A:144:ARG:H	1.80	0.95
1:B:91:GLY:O	1:B:95:THR:HG23	1.66	0.95
1:A:202:SER:O	1:A:205:SER:N	1.99	0.94
1:A:159:ASP:OD1	1:A:162:ARG:N	2.00	0.94
1:B:140:LEU:H	1:B:257:LYS:HZ1	1.06	0.93
1:A:149:VAL:CG1	1:B:319:MET:HE3	1.97	0.93
1:B:42:GLY:HA3	1:B:43:GLN:HB2	1.51	0.92
1:A:140:LEU:O	1:A:142:LYS:N	2.03	0.91
1:B:164:PRO:O	1:B:165:TYR:HB3	1.67	0.91
1:A:295:ASN:HA	1:A:330:THR:O	1.71	0.91
1:A:333:VAL:HG12	1:A:334:ASN:H	1.36	0.90
1:A:199:ASN:O	1:A:203:SER:OG	1.90	0.90
1:B:88:THR:OG1	1:B:237:GLU:OE2	1.90	0.90
1:A:29:PHE:CE1	1:A:31:PRO:HD2	2.08	0.89
1:B:140:LEU:H	1:B:257:LYS:NZ	1.69	0.89
1:A:87:GLN:O	1:A:90:SER:OG	1.88	0.89
1:B:104:GLN:HE21	1:B:104:GLN:HA	1.36	0.89
1:A:266:ILE:CG1	1:A:327:ILE:CD1	2.35	0.88
1:A:284:MET:CE	1:A:288:LEU:HD21	2.04	0.87
1:A:202:SER:O	1:A:204:ARG:N	2.07	0.87
1:A:47:TYR:OH	1:A:315:LYS:CE	2.21	0.87
1:A:201:HIS:O	1:A:205:SER:OG	1.91	0.87
1:A:47:TYR:OH	1:A:315:LYS:CD	2.23	0.87
1:A:141:ASP:OD1	1:A:283:LYS:HE3	1.75	0.86
1:A:20:GLU:HA	1:A:23:ILE:HG22	1.57	0.86
1:A:158:GLU:OE1	1:A:286:ARG:NH2	2.09	0.86
1:A:158:GLU:HA	1:A:163:VAL:O	1.74	0.86
1:A:284:MET:HE3	1:A:288:LEU:HD21	1.56	0.86
1:A:296:CYS:H	1:A:331:VAL:HG12	1.36	0.85
1:A:141:ASP:C	1:A:142:LYS:HD2	1.96	0.85
1:B:74:VAL:HG11	1:B:213:ILE:HD12	1.56	0.85
1:A:49:PHE:HA	1:A:325:LYS:HE3	1.59	0.85
1:A:314:THR:O	1:A:318:LEU:CD2	2.26	0.83
1:A:127:LEU:CA	1:A:217:ASN:HA	2.09	0.83
1:A:28:LYS:HZ1	1:A:28:LYS:H	1.26	0.82
1:A:283:LYS:H	1:A:283:LYS:HD3	1.43	0.82
1:B:83:PHE:HB3	1:B:231:VAL:HB	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HZ3	1:A:308:VAL:H	1.27	0.82
1:B:30:ILE:CG1	1:B:306:PRO:O	2.27	0.82
1:B:30:ILE:HD11	1:B:308:VAL:CA	2.08	0.82
1:A:259:LEU:HD22	1:A:259:LEU:H	1.45	0.82
1:B:40:VAL:C	1:B:41:ILE:HD13	1.99	0.82
1:B:242:THR:HG23	1:B:243:GLY:H	1.42	0.81
1:A:296:CYS:N	1:A:331:VAL:CG1	2.40	0.81
1:B:175:SER:N	1:B:179:GLU:OE1	2.13	0.81
1:A:127:LEU:HA	1:A:217:ASN:HA	1.61	0.81
1:A:319:MET:O	1:A:323:ARG:HG3	1.79	0.81
1:A:266:ILE:HG12	1:A:327:ILE:HD11	1.62	0.81
1:B:14:ARG:HH11	1:B:95:THR:HG22	1.45	0.81
1:A:139:TYR:CD1	1:A:140:LEU:HD22	2.16	0.81
1:A:149:VAL:CG1	1:B:319:MET:CE	2.58	0.80
1:A:288:LEU:HD23	1:A:288:LEU:H	1.46	0.80
1:A:295:ASN:HA	1:A:331:VAL:HA	1.62	0.80
1:A:266:ILE:O	1:A:269:LEU:N	2.15	0.80
1:B:273:THR:HG23	1:B:274:LYS:HG3	1.62	0.80
1:B:242:THR:HG23	1:B:243:GLY:N	1.97	0.79
1:A:282:SER:HB2	1:A:283:LYS:NZ	1.96	0.79
1:A:47:TYR:OH	1:A:315:LYS:NZ	2.13	0.79
1:B:159:ASP:CG	1:B:165:TYR:CE1	2.54	0.79
1:A:174:VAL:CA	1:A:179:GLU:OE1	2.29	0.79
1:B:104:GLN:NE2	1:B:104:GLN:HA	1.94	0.79
1:A:203:SER:O	1:A:204:ARG:NE	2.16	0.78
1:A:287:ILE:HB	1:A:288:LEU:HD23	1.64	0.78
1:A:142:LYS:HD2	1:A:142:LYS:N	1.99	0.77
1:A:172:ARG:NH2	1:A:186:GLU:OE1	2.14	0.77
1:A:148:ASP:OD2	1:A:151:LYS:CD	2.33	0.77
1:A:14:ARG:HH11	1:A:95:THR:CG2	1.94	0.76
1:A:163:VAL:CG2	1:A:164:PRO:HD2	2.15	0.76
1:B:153:ASN:O	1:B:153:ASN:ND2	2.16	0.76
1:A:261:ALA:O	1:A:265:VAL:HG23	1.83	0.76
1:A:266:ILE:HD11	1:A:324:ALA:HA	1.67	0.76
1:B:269:LEU:HB2	1:B:327:ILE:HD13	1.68	0.76
1:A:163:VAL:HG23	1:A:164:PRO:HD2	1.68	0.75
1:B:193:VAL:HG23	1:B:196:THR:N	1.98	0.75
1:B:238:LYS:O	1:B:239:VAL:HG23	1.86	0.75
1:A:172:ARG:HH22	1:A:186:GLU:CD	1.89	0.75
1:B:323:ARG:O	1:B:326:THR:HG23	1.87	0.75
1:A:127:LEU:HA	1:A:216:GLU:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD23	1:A:288:LEU:N	2.02	0.75
1:A:88:THR:OG1	1:A:237:GLU:OE2	2.05	0.75
1:A:279:TYR:HA	1:A:285:THR:CG2	2.17	0.75
1:A:148:ASP:OD2	1:A:151:LYS:HD3	1.87	0.74
1:B:30:ILE:HG12	1:B:306:PRO:O	1.87	0.74
1:B:41:ILE:CD1	1:B:41:ILE:N	2.46	0.74
1:B:5:ALA:HB2	1:B:331:VAL:O	1.88	0.74
1:A:315:LYS:HE2	1:A:319:MET:HG3	1.69	0.74
1:B:58:THR:HG1	1:B:61:GLN:HG3	1.51	0.74
1:B:274:LYS:HZ3	1:B:274:LYS:HB2	1.51	0.73
1:B:127:LEU:HD13	1:B:129:PHE:CE2	2.22	0.73
1:A:283:LYS:H	1:A:283:LYS:CD	1.99	0.73
1:A:283:LYS:N	1:A:283:LYS:HZ2	1.86	0.73
1:B:256:ASN:OD1	1:B:257:LYS:N	2.22	0.73
1:A:149:VAL:H	1:B:319:MET:HE3	1.52	0.73
1:A:6:GLU:OE1	1:A:330:THR:HG23	1.89	0.72
1:A:190:ASN:HD22	1:A:190:ASN:N	1.86	0.72
1:A:173:PHE:HD2	1:B:244:ALA:HB3	1.53	0.72
1:A:83:PHE:HB3	1:A:231:VAL:HB	1.71	0.72
1:B:42:GLY:CA	1:B:43:GLN:CB	2.45	0.71
1:A:148:ASP:O	1:A:151:LYS:HG2	1.91	0.71
1:B:197:ASN:ND2	1:B:200:GLU:CD	2.44	0.71
1:A:173:PHE:HB3	1:B:244:ALA:HB2	1.73	0.71
1:B:126:ASN:H	1:B:126:ASN:HD22	1.39	0.71
1:A:149:VAL:N	1:B:319:MET:HE3	2.05	0.71
1:A:96:MET:CE	1:A:108:ILE:HD12	2.19	0.71
1:A:45:LYS:HD3	1:A:45:LYS:H	1.56	0.71
1:B:30:ILE:CD1	1:B:308:VAL:CB	2.55	0.70
1:B:197:ASN:HD21	1:B:200:GLU:CD	1.94	0.70
1:A:164:PRO:HG3	1:A:286:ARG:O	1.92	0.69
1:B:245:GLU:HG3	1:B:246:GLY:N	2.06	0.69
1:B:63:TYR:CD1	1:B:111:ARG:HB3	2.27	0.69
1:B:127:LEU:CD1	1:B:127:LEU:O	2.38	0.69
1:A:196:THR:N	1:A:197:ASN:HA	2.03	0.68
1:A:265:VAL:HG21	1:A:285:THR:CG2	2.22	0.68
1:A:200:GLU:O	1:A:203:SER:OG	2.11	0.68
1:A:175:SER:N	1:A:179:GLU:OE1	2.25	0.68
1:A:63:TYR:CE1	1:A:67:ALA:HB3	2.27	0.68
1:A:58:THR:O	1:A:62:VAL:HG23	1.94	0.68
1:B:274:LYS:NZ	1:B:274:LYS:HB2	2.09	0.68
1:B:124:ASP:CG	1:B:126:ASN:HD21	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG22	1:B:41:ILE:HG22	1.76	0.68
1:A:116:ILE:HD13	1:A:213:ILE:HD11	1.76	0.68
1:A:266:ILE:O	1:A:269:LEU:HB2	1.93	0.68
1:B:95:THR:O	1:B:108:ILE:HG13	1.93	0.67
1:A:203:SER:C	1:A:204:ARG:HE	1.98	0.67
1:B:191:ARG:HB2	1:B:198:MET:HE1	1.76	0.67
1:B:242:THR:CG2	1:B:243:GLY:H	2.08	0.67
1:B:25:ARG:CD	1:B:27:ASP:OD1	2.41	0.67
1:A:279:TYR:HA	1:A:285:THR:HG22	1.77	0.66
1:A:333:VAL:HG12	1:A:334:ASN:N	2.08	0.66
1:A:294:GLY:O	1:A:296:CYS:N	2.28	0.66
1:A:63:TYR:CD1	1:A:67:ALA:HB3	2.30	0.66
1:A:139:TYR:CD1	1:A:140:LEU:CD2	2.78	0.66
1:A:284:MET:CA	1:A:287:ILE:HG13	2.25	0.66
1:A:28:LYS:HE2	1:A:308:VAL:HB	1.76	0.66
1:B:126:ASN:O	1:B:127:LEU:HG	1.94	0.66
1:A:159:ASP:CG	1:A:163:VAL:HG12	2.16	0.66
1:B:22:GLU:HA	1:B:27:ASP:OD2	1.96	0.66
1:B:290:ASP:O	1:B:294:GLY:O	2.14	0.66
1:A:282:SER:HB2	1:A:283:LYS:HZ1	1.57	0.66
1:A:283:LYS:HG2	1:A:284:MET:N	2.04	0.66
1:A:216:GLU:HG3	1:A:223:LYS:HG2	1.78	0.66
1:B:272:GLY:O	1:B:274:LYS:HD3	1.96	0.66
1:A:124:ASP:OD1	1:A:125:GLU:N	2.29	0.66
1:A:265:VAL:HG21	1:A:285:THR:HG21	1.78	0.66
1:B:102:ASP:OD2	1:B:105:LEU:HD13	1.97	0.65
1:A:157:HIS:O	1:A:164:PRO:CA	2.36	0.65
1:A:278:PRO:HB2	1:A:281:ASP:OD1	1.97	0.65
1:A:139:TYR:C	1:A:140:LEU:HD22	2.17	0.65
1:B:269:LEU:HB2	1:B:327:ILE:CD1	2.26	0.65
1:A:259:LEU:HD22	1:A:259:LEU:N	2.10	0.65
1:B:269:LEU:CB	1:B:327:ILE:HD13	2.26	0.65
1:A:150:SER:O	1:B:45:LYS:HD3	1.95	0.65
1:A:174:VAL:HG12	1:A:179:GLU:HB3	1.78	0.65
1:B:210:LEU:HD12	1:B:211:ILE:H	1.62	0.65
1:A:195:VAL:O	1:A:196:THR:HB	1.96	0.64
1:A:295:ASN:C	1:A:331:VAL:HG12	2.16	0.64
1:A:143:ILE:CD1	1:A:166:VAL:HG13	2.28	0.64
1:A:165:TYR:HE2	1:A:167:LYS:HA	1.62	0.64
1:A:269:LEU:HB3	1:A:327:ILE:HG12	1.79	0.64
1:A:315:LYS:NZ	1:A:319:MET:CG	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG23	1:A:267:SER:N	2.13	0.64
1:B:30:ILE:HG22	1:B:41:ILE:CG2	2.28	0.64
1:A:160:LYS:O	1:A:162:ARG:HG3	1.97	0.64
1:B:272:GLY:O	1:B:273:THR:HG22	1.96	0.64
1:A:202:SER:O	1:A:205:SER:OG	2.16	0.64
1:B:30:ILE:HD11	1:B:308:VAL:N	2.13	0.64
1:A:259:LEU:CD2	1:A:259:LEU:H	2.09	0.64
1:A:266:ILE:HD11	1:A:324:ALA:CB	2.28	0.64
1:B:108:ILE:O	1:B:112:ILE:HG13	1.98	0.64
1:B:20:GLU:O	1:B:24:LEU:HB2	1.97	0.63
1:B:273:THR:C	1:B:274:LYS:HG3	2.19	0.63
1:A:275:THR:HG22	1:A:276:HIS:N	2.12	0.63
1:B:257:LYS:HD3	1:B:258:SER:H	1.62	0.63
1:A:283:LYS:O	1:A:286:ARG:HB3	1.98	0.63
1:A:259:LEU:O	1:A:262:LEU:N	2.31	0.63
1:A:295:ASN:HB2	1:A:332:SER:H	1.63	0.63
1:B:151:LYS:HB3	1:B:154:LEU:HD21	1.79	0.63
1:A:312:ALA:O	1:A:314:THR:N	2.32	0.62
1:B:159:ASP:OD1	1:B:165:TYR:HE1	1.79	0.62
1:A:96:MET:HE1	1:A:108:ILE:HD12	1.80	0.62
1:A:148:ASP:OD2	1:A:151:LYS:HD2	1.99	0.62
1:A:284:MET:HE2	1:A:288:LEU:HD21	1.80	0.62
1:A:140:LEU:HD22	1:A:140:LEU:N	2.13	0.62
1:A:190:ASN:ND2	1:A:190:ASN:N	2.47	0.62
1:A:189:ALA:O	1:A:192:HIS:N	2.32	0.62
1:A:20:GLU:O	1:A:23:ILE:HG22	1.99	0.62
1:A:319:MET:HA	1:A:319:MET:HE3	1.82	0.62
1:B:30:ILE:HB	1:B:31:PRO:CD	2.25	0.62
1:A:126:ASN:C	1:A:127:LEU:HG	2.20	0.62
1:A:290:ASP:CG	1:A:294:GLY:HA3	2.19	0.62
1:A:296:CYS:H	1:A:331:VAL:CG1	2.06	0.61
1:A:317:THR:O	1:A:320:PHE:N	2.31	0.61
1:A:257:LYS:HD3	1:A:258:SER:N	2.16	0.61
1:A:45:LYS:H	1:A:45:LYS:CD	2.11	0.61
1:A:172:ARG:NH2	1:A:186:GLU:CD	2.52	0.61
1:A:20:GLU:HA	1:A:23:ILE:CG2	2.28	0.61
1:A:139:TYR:CG	1:A:140:LEU:CD2	2.83	0.61
1:A:217:ASN:HD21	1:A:222:LYS:HB2	1.63	0.61
1:B:12:MET:HG2	1:B:51:ARG:HB3	1.83	0.61
1:A:127:LEU:O	1:A:127:LEU:HD12	1.99	0.61
1:A:20:GLU:CA	1:A:23:ILE:HG22	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD1	1:A:283:LYS:CE	2.46	0.61
1:B:81:THR:HG23	1:B:229:TYR:HB2	1.83	0.61
1:B:5:ALA:CB	1:B:331:VAL:O	2.48	0.61
1:B:145:ASP:CG	1:B:170:THR:HG23	2.20	0.61
1:B:19:ASN:HD21	1:B:21:ALA:HB3	1.65	0.60
1:B:124:ASP:CG	1:B:126:ASN:ND2	2.54	0.60
1:A:172:ARG:HD2	1:B:240:SER:O	2.01	0.60
1:B:139:TYR:CD1	1:B:140:LEU:HG	2.36	0.60
1:B:200:GLU:O	1:B:204:ARG:CD	2.50	0.60
1:A:139:TYR:CG	1:A:140:LEU:HD22	2.36	0.60
1:A:96:MET:HA	1:A:96:MET:CE	2.31	0.60
1:A:193:VAL:HG23	1:A:193:VAL:O	2.01	0.60
1:B:104:GLN:HE21	1:B:104:GLN:CA	2.11	0.60
1:B:141:ASP:H	1:B:257:LYS:HE3	1.66	0.60
1:B:8:SER:HA	1:B:328:LYS:HA	1.83	0.60
1:A:257:LYS:O	1:A:260:SER:OG	2.20	0.60
1:A:312:ALA:O	1:A:315:LYS:N	2.31	0.60
1:B:161:ASN:O	1:B:162:ARG:HB3	2.02	0.60
1:B:208:ILE:HG13	1:B:231:VAL:HG22	1.83	0.60
1:B:30:ILE:CD1	1:B:308:VAL:CA	2.79	0.60
1:A:266:ILE:HD11	1:A:324:ALA:CA	2.31	0.60
1:B:83:PHE:CB	1:B:231:VAL:HB	2.30	0.60
1:B:18:LEU:HD22	1:B:22:GLU:HB3	1.83	0.59
1:B:242:THR:CG2	1:B:243:GLY:N	2.65	0.59
1:A:283:LYS:HZ3	1:A:284:MET:CB	2.15	0.59
1:A:173:PHE:CD2	1:B:244:ALA:HB3	2.36	0.59
1:A:148:ASP:HB3	1:A:151:LYS:HD3	1.84	0.59
1:A:172:ARG:HD2	1:B:240:SER:C	2.22	0.59
1:A:28:LYS:H	1:A:28:LYS:NZ	1.98	0.59
1:A:317:THR:O	1:A:320:PHE:HB3	2.03	0.59
1:A:143:ILE:CG2	1:A:144:ARG:N	2.43	0.58
1:A:25:ARG:NH1	1:A:27:ASP:OD2	2.36	0.58
1:A:92:LYS:NZ	2:A:501:SO4:S	2.76	0.58
1:A:283:LYS:O	1:A:286:ARG:N	2.36	0.58
1:B:236:SER:C	1:B:238:LYS:H	2.06	0.58
1:B:266:ILE:HD11	1:B:292:LEU:HD22	1.84	0.58
1:B:223:LYS:O	1:B:224:LEU:HD23	2.02	0.58
1:B:295:ASN:HA	1:B:331:VAL:HA	1.83	0.58
1:A:217:ASN:ND2	1:A:222:LYS:HB2	2.18	0.58
1:A:302:ILE:HG13	1:A:302:ILE:O	2.04	0.58
1:A:190:ASN:ND2	1:A:190:ASN:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HA	1:B:216:GLU:O	2.04	0.58
1:A:266:ILE:HG13	1:A:327:ILE:HD13	1.76	0.58
1:B:239:VAL:O	1:B:240:SER:OG	2.22	0.58
1:A:258:SER:O	1:A:261:ALA:HB3	2.04	0.57
1:B:126:ASN:N	1:B:126:ASN:HD22	2.00	0.57
1:A:211:ILE:HG22	1:A:213:ILE:HG13	1.86	0.57
1:B:124:ASP:OD1	1:B:125:GLU:N	2.37	0.57
1:A:295:ASN:CA	1:A:331:VAL:HA	2.32	0.57
1:B:274:LYS:C	1:B:274:LYS:HZ2	1.98	0.57
1:B:245:GLU:CG	1:B:246:GLY:H	2.09	0.57
1:B:290:ASP:OD1	1:B:294:GLY:O	2.22	0.57
1:A:208:ILE:N	1:A:208:ILE:HD12	2.20	0.57
1:B:324:ALA:C	1:B:326:THR:H	2.08	0.57
1:A:283:LYS:HZ3	1:A:284:MET:H	1.52	0.57
1:A:283:LYS:NZ	1:A:284:MET:HB3	2.20	0.57
1:A:148:ASP:HB2	1:A:170:THR:HG21	1.85	0.56
1:B:69:GLN:O	1:B:73:ASP:OD1	2.21	0.56
1:A:141:ASP:O	1:A:283:LYS:HD2	2.05	0.56
1:A:126:ASN:OD1	1:A:127:LEU:HG	2.04	0.56
1:A:275:THR:HG22	1:A:276:HIS:H	1.69	0.56
1:B:191:ARG:HB3	1:B:198:MET:SD	2.46	0.56
1:B:140:LEU:N	1:B:257:LYS:NZ	2.45	0.56
1:B:210:LEU:HD12	1:B:211:ILE:N	2.21	0.56
1:B:193:VAL:HG23	1:B:196:THR:HG23	1.87	0.56
1:B:47:TYR:CE2	1:B:318:LEU:HD23	2.41	0.56
1:A:319:MET:HA	1:A:319:MET:CE	2.35	0.56
1:B:41:ILE:HD11	1:B:47:TYR:HD2	1.69	0.56
1:A:165:TYR:HD2	1:A:166:VAL:O	1.89	0.56
1:B:159:ASP:OD1	1:B:165:TYR:CZ	2.58	0.56
1:B:190:ASN:O	1:B:192:HIS:N	2.39	0.56
1:B:200:GLU:O	1:B:204:ARG:HD2	2.06	0.56
1:B:81:THR:OG1	1:B:296:CYS:SG	2.61	0.56
1:A:23:ILE:HG23	1:A:24:LEU:N	2.21	0.56
1:A:25:ARG:HG2	1:A:25:ARG:O	2.05	0.56
1:A:172:ARG:HD3	1:B:241:LYS:HB3	1.88	0.56
1:A:110:PRO:O	1:A:113:ALA:HB3	2.06	0.56
1:A:266:ILE:HG23	1:A:267:SER:H	1.71	0.56
1:A:263:GLY:O	1:A:266:ILE:HG22	2.05	0.55
1:A:279:TYR:HA	1:A:285:THR:HG21	1.87	0.55
1:A:189:ALA:O	1:A:191:ARG:N	2.39	0.55
1:B:103:PRO:C	1:B:104:GLN:HE21	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:CD	1:B:258:SER:H	2.19	0.55
1:B:30:ILE:HG13	1:B:307:SER:C	2.26	0.55
1:A:29:PHE:CE1	1:A:31:PRO:CD	2.87	0.55
1:A:38:THR:HG22	1:A:48:VAL:HG22	1.86	0.55
1:A:177:PRO:O	1:A:181:MET:HG2	2.06	0.55
1:B:29:PHE:C	1:B:30:ILE:HG12	2.27	0.55
1:A:172:ARG:HG3	1:A:173:PHE:N	2.22	0.55
1:A:295:ASN:CA	1:A:330:THR:O	2.50	0.55
1:A:312:ALA:O	1:A:313:GLU:C	2.45	0.54
1:B:274:LYS:O	1:B:275:THR:CG2	2.48	0.54
1:B:164:PRO:HG2	1:B:289:GLN:OE1	2.07	0.54
1:A:259:LEU:O	1:A:262:LEU:HB3	2.06	0.54
1:A:287:ILE:C	1:A:289:GLN:H	2.11	0.54
1:A:148:ASP:CG	1:A:151:LYS:HD3	2.28	0.54
1:A:141:ASP:OD1	1:A:283:LYS:CD	2.55	0.54
1:B:8:SER:HB3	1:B:328:LYS:HG2	1.88	0.54
1:A:96:MET:HA	1:A:96:MET:HE2	1.89	0.54
1:B:283:LYS:O	1:B:286:ARG:HB2	2.07	0.54
1:B:74:VAL:HG11	1:B:213:ILE:CD1	2.32	0.54
1:A:37:GLU:HB2	1:A:49:PHE:O	2.08	0.54
1:B:16:ARG:NH2	1:B:305:SER:OG	2.41	0.54
1:A:159:ASP:OD2	1:A:163:VAL:HG12	2.08	0.54
1:A:163:VAL:HG22	1:A:164:PRO:HD2	1.87	0.54
1:A:296:CYS:CA	1:A:331:VAL:HG12	2.36	0.53
1:B:196:THR:O	1:B:197:ASN:HB3	2.08	0.53
1:B:323:ARG:O	1:B:326:THR:CG2	2.55	0.53
1:B:45:LYS:O	1:B:46:PRO:C	2.47	0.53
1:A:206:HIS:HB3	1:A:233:LEU:HA	1.90	0.53
1:A:148:ASP:CB	1:A:151:LYS:HD3	2.38	0.53
1:B:145:ASP:OD2	1:B:170:THR:HG23	2.07	0.53
1:B:198:MET:O	1:B:201:HIS:N	2.39	0.53
1:A:259:LEU:O	1:A:263:GLY:N	2.38	0.53
1:B:164:PRO:O	1:B:165:TYR:CB	2.48	0.53
1:A:63:TYR:CE1	1:A:67:ALA:CB	2.91	0.53
1:A:284:MET:O	1:A:287:ILE:HG13	2.08	0.53
1:B:29:PHE:O	1:B:30:ILE:HG12	2.09	0.53
1:A:284:MET:HE2	1:A:288:LEU:HD11	1.89	0.53
1:B:30:ILE:HG13	1:B:306:PRO:O	2.08	0.53
1:A:34:LYS:O	1:A:38:THR:OG1	2.19	0.52
1:A:173:PHE:HB3	1:B:244:ALA:CB	2.37	0.52
1:A:163:VAL:CG2	1:A:164:PRO:CD	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HZ1	1:A:28:LYS:N	2.00	0.52
1:B:41:ILE:O	1:B:43:GLN:HB3	2.09	0.52
1:B:14:ARG:HH11	1:B:95:THR:CG2	2.20	0.52
1:B:160:LYS:HG3	1:B:161:ASN:N	2.23	0.52
1:B:238:LYS:O	1:B:239:VAL:CG2	2.57	0.52
1:B:59:GLN:HG2	1:B:106:MET:O	2.10	0.52
1:A:120:ILE:CD1	1:A:131:ILE:HD11	2.40	0.52
1:A:266:ILE:O	1:A:269:LEU:CB	2.58	0.52
1:A:198:MET:HE3	1:A:199:ASN:HA	1.92	0.51
1:B:159:ASP:CG	1:B:165:TYR:CD1	2.83	0.51
1:B:223:LYS:NZ	1:B:337:HIS:HB3	2.26	0.51
1:B:14:ARG:NH1	1:B:95:THR:HG22	2.22	0.51
1:A:126:ASN:O	1:A:127:LEU:HG	2.10	0.51
1:B:29:PHE:CE1	1:B:31:PRO:HD2	2.45	0.51
1:A:43:GLN:HE21	1:A:44:GLY:N	2.08	0.51
1:A:47:TYR:OH	1:A:315:LYS:HD2	2.08	0.51
1:B:163:VAL:O	1:B:164:PRO:O	2.28	0.51
1:B:256:ASN:O	1:B:260:SER:OG	2.26	0.51
1:B:191:ARG:O	1:B:198:MET:CE	2.59	0.50
1:A:145:ASP:OD1	1:A:147:LEU:N	2.42	0.50
1:A:198:MET:C	1:A:198:MET:HE3	2.32	0.50
1:A:283:LYS:NZ	1:A:284:MET:CB	2.75	0.50
1:A:284:MET:O	1:A:288:LEU:HD23	2.11	0.50
1:A:6:GLU:O	1:A:6:GLU:HG3	2.10	0.50
1:B:273:THR:O	1:B:274:LYS:HG3	2.11	0.50
1:B:10:LYS:O	1:B:299:THR:HA	2.10	0.50
1:A:266:ILE:CG2	1:A:267:SER:H	2.25	0.50
1:A:266:ILE:CG2	1:A:267:SER:N	2.75	0.50
1:A:41:ILE:N	1:A:41:ILE:HD12	2.26	0.50
1:A:283:LYS:O	1:A:287:ILE:HG13	2.12	0.50
1:A:161:ASN:C	1:A:162:ARG:HG3	2.32	0.49
1:B:144:ARG:NH2	1:B:191:ARG:HA	2.27	0.49
1:A:269:LEU:HD13	1:A:277:VAL:HG11	1.94	0.49
1:A:284:MET:C	1:A:287:ILE:HG13	2.33	0.49
1:A:265:VAL:HG21	1:A:285:THR:HG23	1.91	0.49
1:B:145:ASP:OD1	1:B:170:THR:HG23	2.13	0.49
1:B:41:ILE:HD11	1:B:47:TYR:CD2	2.47	0.49
1:B:73:ASP:OD2	1:B:297:ARG:HD2	2.13	0.49
1:A:165:TYR:CE2	1:A:167:LYS:HA	2.45	0.49
1:B:241:LYS:HG3	1:B:241:LYS:O	2.11	0.49
1:A:119:HIS:O	1:A:122:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HB3	1:A:217:ASN:CB	2.42	0.49
1:A:189:ALA:C	1:A:191:ARG:N	2.66	0.49
1:B:256:ASN:O	1:B:257:LYS:C	2.51	0.49
1:A:83:PHE:CB	1:A:231:VAL:HB	2.42	0.49
1:B:200:GLU:HB3	1:B:204:ARG:CZ	2.42	0.49
1:A:23:ILE:CG2	1:A:24:LEU:N	2.75	0.49
1:A:189:ALA:C	1:A:191:ARG:H	2.16	0.48
1:A:193:VAL:CG2	1:A:193:VAL:O	2.61	0.48
1:A:296:CYS:C	1:A:331:VAL:HG11	2.33	0.48
1:A:49:PHE:CZ	1:A:318:LEU:HD12	2.49	0.48
1:B:92:LYS:NZ	2:B:401:SO4:O3	2.47	0.48
1:A:283:LYS:NZ	1:A:284:MET:H	2.12	0.48
1:A:283:LYS:NZ	1:A:284:MET:N	2.62	0.48
1:B:272:GLY:C	1:B:274:LYS:H	2.16	0.48
1:A:139:TYR:CE1	1:A:140:LEU:HD21	2.48	0.48
1:A:18:LEU:CD2	1:A:307:SER:HB2	2.44	0.48
1:B:8:SER:HA	1:B:327:ILE:O	2.14	0.48
1:A:204:ARG:CA	1:A:204:ARG:HE	2.27	0.48
1:B:207:SER:C	1:B:208:ILE:HD12	2.34	0.48
1:B:92:LYS:HB2	2:B:401:SO4:O4	2.14	0.48
1:A:40:VAL:C	1:A:41:ILE:HD12	2.34	0.48
1:B:127:LEU:HD13	1:B:129:PHE:HE2	1.76	0.48
1:A:283:LYS:HZ3	1:A:284:MET:N	2.11	0.47
1:B:133:VAL:HG12	1:B:211:ILE:HG12	1.96	0.47
1:B:18:LEU:HD22	1:B:22:GLU:CB	2.44	0.47
1:A:320:PHE:CD2	1:A:320:PHE:C	2.88	0.47
1:A:266:ILE:CD1	1:A:324:ALA:HB2	2.45	0.47
1:A:127:LEU:N	1:A:217:ASN:HA	2.29	0.47
1:A:156:VAL:HG12	1:A:157:HIS:N	2.30	0.47
1:A:229:TYR:O	1:A:230:LEU:HD23	2.14	0.47
1:A:38:THR:CG2	1:A:48:VAL:HG22	2.44	0.47
1:B:268:ALA:HB3	1:B:277:VAL:HG13	1.96	0.47
1:B:88:THR:OG1	1:B:237:GLU:CD	2.52	0.47
1:B:18:LEU:HG	1:B:306:PRO:HG2	1.97	0.47
1:B:41:ILE:O	1:B:44:GLY:N	2.39	0.47
1:A:179:GLU:O	1:A:183:VAL:HG23	2.14	0.47
1:A:99:LYS:N	1:A:99:LYS:HE3	2.30	0.47
1:B:140:LEU:O	1:B:142:LYS:N	2.48	0.47
1:B:63:TYR:CD1	1:B:111:ARG:CB	2.97	0.47
1:A:14:ARG:CZ	1:A:62:VAL:HG21	2.44	0.47
1:B:43:GLN:HG3	1:B:44:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HA	1:A:217:ASN:CA	2.39	0.47
1:B:200:GLU:O	1:B:204:ARG:CG	2.63	0.47
1:A:158:GLU:HB3	1:A:162:ARG:HA	1.97	0.47
1:A:129:PHE:CD2	1:A:215:GLN:HB3	2.50	0.46
1:B:200:GLU:O	1:B:204:ARG:HG3	2.15	0.46
1:B:192:HIS:CD2	1:B:192:HIS:C	2.89	0.46
1:B:272:GLY:O	1:B:274:LYS:CD	2.61	0.46
1:A:269:LEU:HD23	1:A:327:ILE:HD13	1.98	0.46
1:A:74:VAL:HG11	1:A:213:ILE:HD12	1.98	0.46
1:A:282:SER:O	1:A:285:THR:HB	2.16	0.46
1:A:59:GLN:OE1	1:A:94:HIS:O	2.33	0.46
1:B:127:LEU:CD1	1:B:129:PHE:CE2	2.97	0.46
1:A:151:LYS:H	1:A:151:LYS:HG2	1.48	0.46
1:B:15:PHE:CD1	1:B:304:CYS:HB2	2.51	0.46
1:B:39:VAL:HG13	1:B:47:TYR:HB2	1.96	0.46
1:A:28:LYS:HZ3	1:A:308:VAL:N	2.06	0.46
1:A:266:ILE:CD1	1:A:327:ILE:CD1	2.94	0.46
1:A:127:LEU:HB3	1:A:217:ASN:CA	2.46	0.46
1:A:43:GLN:NE2	1:A:44:GLY:H	2.13	0.46
1:A:148:ASP:CG	1:A:151:LYS:CD	2.83	0.46
1:A:174:VAL:HG12	1:A:179:GLU:CB	2.46	0.46
1:A:178:GLU:O	1:A:181:MET:HB2	2.16	0.46
1:A:149:VAL:HG12	1:B:319:MET:SD	2.56	0.46
1:B:191:ARG:O	1:B:198:MET:HE2	2.15	0.46
1:A:143:ILE:HD13	1:A:166:VAL:CG1	2.46	0.46
1:A:283:LYS:N	1:A:283:LYS:CD	2.73	0.46
1:A:290:ASP:O	1:A:294:GLY:N	2.49	0.46
1:A:190:ASN:HD21	1:B:323:ARG:CD	2.29	0.45
1:A:163:VAL:HG22	1:A:164:PRO:CD	2.47	0.45
1:A:165:TYR:C	1:A:165:TYR:CD2	2.89	0.45
1:A:269:LEU:HB3	1:A:327:ILE:CG1	2.45	0.45
1:B:110:PRO:O	1:B:113:ALA:HB3	2.17	0.45
1:B:274:LYS:NZ	1:B:274:LYS:CB	2.79	0.45
1:A:269:LEU:HD23	1:A:327:ILE:HG21	1.98	0.45
1:B:124:ASP:OD1	1:B:126:ASN:ND2	2.49	0.45
1:B:210:LEU:HD22	1:B:229:TYR:CE1	2.52	0.45
1:B:324:ALA:O	1:B:326:THR:N	2.48	0.45
1:A:6:GLU:HA	1:A:329:ASN:O	2.17	0.45
1:A:74:VAL:HA	1:A:78:TYR:O	2.16	0.45
1:B:126:ASN:O	1:B:127:LEU:CG	2.61	0.45
1:B:30:ILE:CG2	1:B:41:ILE:HG22	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:NE	1:A:204:ARG:CA	2.78	0.45
1:A:145:ASP:HB3	1:A:151:LYS:HG3	1.99	0.45
1:A:319:MET:CA	1:A:319:MET:CE	2.94	0.45
1:B:135:TYR:HD1	1:B:208:ILE:O	1.99	0.45
1:B:215:GLN:HG2	1:B:224:LEU:HB2	1.99	0.45
1:B:257:LYS:CG	1:B:258:SER:H	2.29	0.45
1:B:325:LYS:O	1:B:325:LYS:HG2	2.17	0.45
1:B:91:GLY:O	1:B:95:THR:CG2	2.52	0.45
1:A:139:TYR:O	1:A:140:LEU:O	2.34	0.45
1:A:139:TYR:C	1:A:140:LEU:CD2	2.83	0.45
1:B:74:VAL:CG1	1:B:213:ILE:HD12	2.38	0.45
1:A:190:ASN:ND2	1:B:323:ARG:HG2	2.32	0.45
1:A:283:LYS:CG	1:A:284:MET:H	2.09	0.44
1:B:235:GLY:HA3	1:B:237:GLU:OE2	2.17	0.44
1:A:283:LYS:HZ3	1:A:284:MET:HB2	1.83	0.44
1:B:127:LEU:CD1	1:B:129:PHE:HE2	2.29	0.44
1:A:172:ARG:NH2	1:A:186:GLU:OE2	2.51	0.44
1:A:311:GLU:O	1:A:314:THR:HB	2.18	0.44
1:A:28:LYS:CD	1:A:30:ILE:CD1	2.95	0.44
1:B:4:PRO:O	1:B:5:ALA:HB2	2.17	0.44
1:A:159:ASP:OD1	1:A:163:VAL:HG12	2.17	0.44
1:A:204:ARG:HA	1:A:204:ARG:HE	1.82	0.44
1:B:158:GLU:HG3	1:B:162:ARG:O	2.18	0.44
1:A:198:MET:HE3	1:A:202:SER:OG	2.18	0.44
1:B:38:THR:HG22	1:B:48:VAL:HG22	2.00	0.44
1:B:184:ILE:HG13	1:B:209:PHE:CE1	2.53	0.43
1:B:313:GLU:O	1:B:314:THR:C	2.56	0.43
1:A:28:LYS:N	1:A:28:LYS:NZ	2.64	0.43
1:A:49:PHE:HZ	1:A:318:LEU:HD12	1.84	0.43
1:B:236:SER:C	1:B:238:LYS:N	2.70	0.43
1:A:13:CYS:HB2	1:A:302:ILE:HD11	2.00	0.43
1:A:204:ARG:NE	1:A:204:ARG:HA	2.33	0.43
1:A:266:ILE:HD11	1:A:324:ALA:HB2	2.00	0.43
1:A:275:THR:CG2	1:A:276:HIS:N	2.80	0.43
1:A:30:ILE:HD11	1:A:308:VAL:HB	1.99	0.43
1:B:208:ILE:HD12	1:B:208:ILE:N	2.33	0.43
1:A:28:LYS:HE2	1:A:308:VAL:CB	2.44	0.43
1:A:80:GLY:O	1:A:228:LEU:HA	2.17	0.43
1:A:137:GLU:CD	1:A:201:HIS:HE2	2.22	0.43
1:A:237:GLU:HA	1:A:313:GLU:OE1	2.19	0.43
1:B:191:ARG:CB	1:B:198:MET:HE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:O	1:B:245:GLU:HB3	2.19	0.43
1:B:261:ALA:O	1:B:265:VAL:HG23	2.17	0.43
1:B:25:ARG:CZ	1:B:27:ASP:OD2	2.67	0.43
1:B:68:LYS:HB3	1:B:68:LYS:HE3	1.89	0.43
1:A:201:HIS:C	1:A:201:HIS:CD2	2.92	0.43
1:A:131:ILE:HG12	1:A:213:ILE:HG12	2.00	0.43
1:A:284:MET:HA	1:A:287:ILE:HG13	1.97	0.43
1:A:41:ILE:CD1	1:A:41:ILE:N	2.81	0.43
1:B:20:GLU:O	1:B:24:LEU:CB	2.66	0.43
1:A:127:LEU:HB3	1:A:217:ASN:HA	2.01	0.43
1:A:148:ASP:CB	1:A:170:THR:HG21	2.48	0.43
1:A:127:LEU:CB	1:A:217:ASN:HA	2.47	0.43
1:A:312:ALA:C	1:A:314:THR:N	2.72	0.43
1:A:217:ASN:OD1	1:A:217:ASN:O	2.36	0.43
1:A:315:LYS:HE3	1:A:315:LYS:O	2.18	0.43
1:B:109:ILE:N	1:B:110:PRO:HD2	2.34	0.43
1:A:19:ASN:CG	1:A:22:GLU:OE1	2.57	0.43
1:A:284:MET:O	1:A:287:ILE:N	2.49	0.43
1:A:290:ASP:O	1:A:294:GLY:CA	2.66	0.43
1:B:19:ASN:ND2	1:B:21:ALA:HB3	2.34	0.43
1:B:239:VAL:C	1:B:240:SER:OG	2.56	0.43
1:B:140:LEU:N	1:B:257:LYS:HZ1	1.91	0.43
1:A:149:VAL:O	1:A:150:SER:C	2.57	0.43
1:A:80:GLY:HA2	1:A:297:ARG:O	2.19	0.43
1:A:47:TYR:HH	1:A:315:LYS:CD	2.27	0.43
1:A:32:LYS:HB2	1:A:40:VAL:HB	2.01	0.43
1:B:324:ALA:C	1:B:326:THR:N	2.72	0.43
1:A:108:ILE:O	1:A:112:ILE:HG13	2.19	0.42
1:A:277:VAL:HA	1:A:278:PRO:HD3	1.94	0.42
1:A:28:LYS:HE2	1:A:308:VAL:CG1	2.48	0.42
1:A:117:PHE:HB2	1:A:177:PRO:HG3	2.00	0.42
1:B:102:ASP:O	1:B:106:MET:HB3	2.19	0.42
1:A:47:TYR:HH	1:A:315:LYS:HD3	1.83	0.42
1:B:334:ASN:N	1:B:334:ASN:OD1	2.43	0.42
1:A:142:LYS:CD	1:A:142:LYS:N	2.77	0.42
1:A:198:MET:C	1:A:198:MET:SD	2.98	0.42
1:A:20:GLU:O	1:A:21:ALA:C	2.56	0.42
1:B:163:VAL:HG23	1:B:163:VAL:O	2.19	0.42
1:A:153:ASN:N	1:A:153:ASN:OD1	2.52	0.42
1:A:283:LYS:O	1:A:287:ILE:N	2.53	0.42
1:A:315:LYS:O	1:A:319:MET:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PHE:CD1	1:B:31:PRO:HD2	2.54	0.42
1:B:64:ASN:HA	1:B:68:LYS:HB2	2.01	0.42
1:B:120:ILE:HG23	1:B:129:PHE:CD2	2.55	0.42
1:B:146:LEU:HB3	1:B:187:GLY:HA2	2.02	0.42
1:B:238:LYS:O	1:B:239:VAL:CB	2.68	0.42
1:A:198:MET:HE3	1:A:199:ASN:CA	2.50	0.42
1:A:264:ASN:O	1:A:266:ILE:N	2.53	0.42
1:B:236:SER:O	1:B:238:LYS:N	2.52	0.42
1:B:284:MET:C	1:B:286:ARG:N	2.72	0.42
1:B:338:HIS:CG	1:B:338:HIS:O	2.71	0.42
1:A:120:ILE:O	1:A:122:SER:N	2.53	0.42
1:A:282:SER:HB2	1:A:283:LYS:CE	2.49	0.42
1:A:282:SER:C	1:A:283:LYS:HZ2	2.23	0.42
1:B:272:GLY:C	1:B:274:LYS:N	2.73	0.42
1:B:337:HIS:CD2	1:B:337:HIS:H	2.35	0.42
1:A:120:ILE:HA	1:A:123:MET:HE3	2.02	0.42
1:B:280:ARG:HG2	1:B:286:ARG:HD3	2.02	0.42
1:B:308:VAL:C	1:B:310:ASN:N	2.73	0.42
1:A:79:ASN:ND2	1:A:226:GLY:HA2	2.35	0.41
1:B:158:GLU:HA	1:B:164:PRO:HA	2.03	0.41
1:B:128:GLU:OE2	1:B:130:HIS:CE1	2.73	0.41
1:A:140:LEU:O	1:A:142:LYS:HD2	2.21	0.41
1:A:143:ILE:CD1	1:A:166:VAL:CG1	2.98	0.41
1:A:25:ARG:CG	1:A:25:ARG:O	2.68	0.41
1:A:314:THR:HG22	1:A:318:LEU:HD23	2.02	0.41
1:B:131:ILE:HG22	1:B:174:VAL:CG2	2.50	0.41
1:A:232:ASP:OD1	1:A:232:ASP:C	2.59	0.41
1:A:266:ILE:CD1	1:A:327:ILE:HD12	2.51	0.41
1:B:273:THR:C	1:B:274:LYS:CG	2.89	0.41
1:B:30:ILE:HG13	1:B:307:SER:O	2.21	0.41
1:A:139:TYR:CZ	1:A:140:LEU:HD21	2.55	0.41
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.83	0.41
1:A:11:VAL:O	1:A:50:ASP:HB2	2.20	0.41
1:A:146:LEU:HA	1:A:146:LEU:HD23	1.77	0.41
1:A:30:ILE:N	1:A:31:PRO:CD	2.83	0.41
1:B:126:ASN:ND2	1:B:126:ASN:N	2.64	0.41
1:B:21:ALA:O	1:B:22:GLU:C	2.59	0.41
1:A:12:MET:O	1:A:302:ILE:HG12	2.20	0.41
1:A:279:TYR:CE2	1:A:289:GLN:HG3	2.56	0.41
1:B:275:THR:O	1:B:276:HIS:HB3	2.21	0.41
1:B:90:SER:OG	1:B:303:CYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:O	1:B:311:GLU:C	2.59	0.41
1:B:16:ARG:O	1:B:306:PRO:HG3	2.21	0.41
1:A:43:GLN:NE2	1:A:44:GLY:N	2.68	0.41
1:A:32:LYS:NZ	3:A:602:HOH:O	2.50	0.40
1:B:30:ILE:CB	1:B:31:PRO:HD3	2.29	0.40
1:A:63:TYR:HE1	1:A:112:ILE:HG12	1.85	0.40
1:A:159:ASP:OD1	1:A:163:VAL:N	2.54	0.40
1:A:269:LEU:CD1	1:A:277:VAL:HG11	2.51	0.40
1:A:141:ASP:HB3	1:A:142:LYS:CE	2.51	0.40
1:A:24:LEU:C	1:A:26:GLY:H	2.25	0.40
1:A:25:ARG:HH12	1:A:309:PHE:HB2	1.86	0.40
1:A:14:ARG:O	1:A:303:CYS:HA	2.21	0.40
1:B:282:SER:O	1:B:286:ARG:HG3	2.21	0.40
1:B:86:GLY:N	1:B:92:LYS:HD3	2.36	0.40
1:A:198:MET:HE3	1:A:199:ASN:N	2.36	0.40
1:B:274:LYS:HD3	1:B:274:LYS:O	2.21	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	304/341 (89%)	225 (74%)	59 (19%)	20 (7%)	<b>1</b> <b>3</b>
1	B	318/341 (93%)	248 (78%)	43 (14%)	27 (8%)	<b>1</b> <b>1</b>
All	All	622/682 (91%)	473 (76%)	102 (16%)	47 (8%)	<b>1</b> <b>2</b>

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	196	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	198	MET
1	A	203	SER
1	A	295	ASN
1	A	312	ALA
1	A	333	VAL
1	B	5	ALA
1	B	43	GLN
1	B	141	ASP
1	B	164	PRO
1	B	165	TYR
1	B	239	VAL
1	B	245	GLU
1	B	257	LYS
1	B	272	GLY
1	B	274	LYS
1	B	275	THR
1	B	309	PHE
1	A	159	ASP
1	A	190	ASN
1	A	202	SER
1	A	235	GLY
1	A	284	MET
1	A	313	GLU
1	B	17	PRO
1	B	44	GLY
1	B	191	ARG
1	B	240	SER
1	B	325	LYS
1	A	27	ASP
1	A	127	LEU
1	A	140	LEU
1	B	29	PHE
1	B	30	ILE
1	B	124	ASP
1	B	237	GLU
1	B	276	HIS
1	A	121	TYR
1	A	144	ARG
1	B	159	ASP
1	B	160	LYS
1	B	218	VAL
1	A	25	ARG

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Mol	Chain	Res	Type
1	B	295	ASN
1	B	187	GLY
1	A	26	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	275/301 (91%)	233 (85%)	42 (15%)	<b>2</b> <b>7</b>
1	B	287/301 (95%)	252 (88%)	35 (12%)	<b>5</b> <b>13</b>
All	All	562/602 (93%)	485 (86%)	77 (14%)	<b>3</b> <b>9</b>

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	28	LYS
1	A	45	LYS
1	A	51	ARG
1	A	66	CYS
1	A	70	ILE
1	A	87	GLN
1	A	88	THR
1	A	90	SER
1	A	99	LYS
1	A	105	LEU
1	A	134	SER
1	A	140	LEU
1	A	151	LYS
1	A	152	THR
1	A	153	ASN
1	A	158	GLU
1	A	162	ARG
1	A	165	TYR
1	A	170	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	188	LYS
1	A	193	VAL
1	A	198	MET
1	A	200	GLU
1	A	202	SER
1	A	203	SER
1	A	204	ARG
1	A	205	SER
1	A	206	HIS
1	A	220	THR
1	A	257	LYS
1	A	269	LEU
1	A	271	GLU
1	A	280	ARG
1	A	283	LYS
1	A	288	LEU
1	A	310	ASN
1	A	315	LYS
1	A	329	ASN
1	A	330	THR
1	A	332	SER
1	A	334	ASN
1	B	12	MET
1	B	28	LYS
1	B	34	LYS
1	B	38	THR
1	B	40	VAL
1	B	41	ILE
1	B	51	ARG
1	B	57	THR
1	B	58	THR
1	B	68	LYS
1	B	95	THR
1	B	104	GLN
1	B	126	ASN
1	B	127	LEU
1	B	139	TYR
1	B	140	LEU
1	B	149	VAL
1	B	153	ASN
1	B	162	ARG
1	B	170	THR

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Mol	Chain	Res	Type
1	B	219	GLU
1	B	221	GLU
1	B	237	GLU
1	B	240	SER
1	B	241	LYS
1	B	257	LYS
1	B	259	LEU
1	B	274	LYS
1	B	284	MET
1	B	288	LEU
1	B	291	SER
1	B	295	ASN
1	B	318	LEU
1	B	334	ASN
1	B	335	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	79	ASN
1	A	130	HIS
1	A	190	ASN
1	A	329	ASN
1	A	334	ASN
1	B	104	GLN
1	B	126	ASN
1	B	130	HIS
1	B	190	ASN
1	B	192	HIS
1	B	197	ASN
1	B	329	ASN
1	B	335	HIS
1	B	337	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	SO4	A	501	-	4,4,4	0.42	0	6,6,6	0.55	0
2	SO4	B	401	-	4,4,4	0.48	0	6,6,6	1.01	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	B	401	SO4	2	0

## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	310/341 (90%)	0.25	25 (8%) 12 8	58, 104, 158, 207	1 (0%)
1	B	324/341 (95%)	0.05	17 (5%) 27 22	60, 91, 149, 170	1 (0%)
All	All	634/682 (92%)	0.15	42 (6%) 18 14	58, 96, 153, 207	2 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	5.8
1	A	196	THR	5.5
1	A	334	ASN	5.2
1	A	7	CYS	4.7
1	A	161	ASN	4.4
1	B	242	THR	4.3
1	B	28	LYS	4.2
1	A	195	VAL	4.2
1	B	4	PRO	4.2
1	A	197	ASN	3.9
1	A	295	ASN	3.7
1	B	243	GLY	3.5
1	B	161	ASN	3.4
1	A	223	LYS	3.3
1	B	196	THR	3.2
1	B	42	GLY	3.1
1	A	199	ASN	3.1
1	A	162	ARG	3.0
1	A	275	THR	2.9
1	A	13	CYS	2.9
1	B	337	HIS	2.9
1	B	197	ASN	2.9
1	A	6	GLU	2.8
1	A	160	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	276	HIS	2.8
1	A	315	LYS	2.8
1	A	274	LYS	2.7
1	A	219	GLU	2.7
1	A	331	VAL	2.5
1	B	273	THR	2.5
1	B	198	MET	2.5
1	B	200	GLU	2.4
1	B	241	LYS	2.4
1	B	336	HIS	2.3
1	A	194	ALA	2.3
1	A	238	LYS	2.2
1	A	220	THR	2.2
1	B	167	LYS	2.2
1	A	5	ALA	2.2
1	A	198	MET	2.0
1	A	332	SER	2.0
1	B	272	GLY	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	A	501	5/5	0.96	0.09	73,81,85,93	0
2	SO4	B	401	5/5	0.96	0.10	64,65,78,89	0

## 6.5 Other polymers

There are no such residues in this entry.