



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CH7  
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF A BACTERIAL CHEMORECEPTOR FROM THERMOTOGA MARITIMA  
Authors : Park, S.Y.; Bilwes, A.M.; Crane, B.R.  
Deposited on : 2006-03-13  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

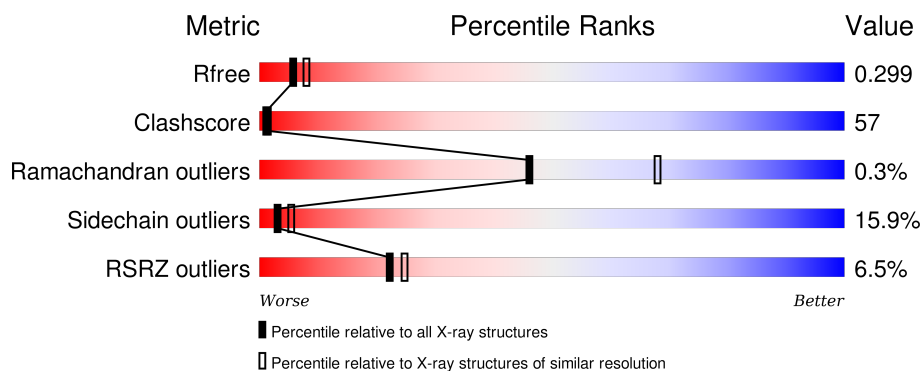
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	<div> <div>7%</div> <div>40%</div> <div>51%</div> <div>8%</div> </div>
2	B	309	<div> <div>6%</div> <div>40%</div> <div>51%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5216 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 METHYL-ACCEPTING CHEMOTAXIS PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2329	1408	406	509	6			

- Molecule 2 is a protein called METHYL-ACCEPTING CHEMOTAXIS PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	1
			2301	1389	402	505	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	466	ASN	THR	CONFLICT	UNP Q9X0M7

- Molecule 3 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Pb	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	266	Total	O	0	0
			266	266		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	24.60 Å 99.40 Å 117.20 Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.30 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-2.50) 95.7 (29.30-2.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.297 0.261 , 0.299	Depositor DCC
$R_{free}$ test set	1859 reflections (11.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 68.3	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 37669 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.44	0/2335	0.61	0/3148
2	B	0.46	1/2306 (0.0%)	0.62	0/3114
All	All	0.45	1/4641 (0.0%)	0.62	0/6262

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	224	MET	C-O	5.01	1.32	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2329	0	2305	288	0
2	B	2301	0	2263	286	0
3	A	2	0	0	0	0
4	A	318	0	0	166	1
4	B	266	0	0	169	1
All	All	5216	0	4568	528	1

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 57.

All (528) 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:408:GLU:HB3	4:A:2236:HOH:O	1.43	1.19
2:B:342:GLY:HA3	4:B:2114:HOH:O	1.38	1.19
1:A:355:ALA:HB2	4:A:2163:HOH:O	1.43	1.18
2:B:261:ASN:HB3	4:B:2034:HOH:O	1.41	1.17
1:A:390:LYS:HB3	4:A:2212:HOH:O	1.46	1.15
1:A:279:GLY:HA2	4:A:2040:HOH:O	1.46	1.14
2:B:246:GLU:HB2	4:B:2010:HOH:O	1.46	1.14
1:A:449:GLU:HB3	4:A:2260:HOH:O	1.47	1.13
2:B:319:ILE:HD11	4:B:2079:HOH:O	1.47	1.12
2:B:393:GLU:HG3	4:B:2144:HOH:O	1.48	1.12
2:B:463:GLU:HA	4:B:2216:HOH:O	1.46	1.12
1:A:354:ASN:HB3	4:A:2170:HOH:O	1.47	1.11
1:A:390:LYS:HA	4:A:2215:HOH:O	1.48	1.11
4:A:2020:HOH:O	2:B:496:ARG:HD3	1.49	1.11
1:A:467:ALA:HB3	4:A:2273:HOH:O	1.51	1.10
4:A:2270:HOH:O	2:B:290:ILE:HD11	1.50	1.09
2:B:361:ASN:HA	4:B:2143:HOH:O	1.53	1.08
2:B:350:VAL:HG22	4:B:2181:HOH:O	1.52	1.08
1:A:318:VAL:HG11	4:B:2203:HOH:O	1.53	1.07
4:A:2063:HOH:O	2:B:454:MET:HG3	1.54	1.07
2:B:298:ALA:HA	4:B:2212:HOH:O	1.55	1.06
2:B:374:ALA:HB3	4:B:2156:HOH:O	1.55	1.05
1:A:430:GLY:HA2	4:A:2250:HOH:O	1.57	1.05
2:B:239:GLU:HG3	4:B:2008:HOH:O	1.56	1.05
2:B:346:ILE:HB	4:B:2120:HOH:O	1.55	1.05
1:A:319:ILE:HG22	4:A:2251:HOH:O	1.53	1.04
2:B:526:ALA:HB1	4:B:2260:HOH:O	1.56	1.02
1:A:330:LYS:HA	4:A:2112:HOH:O	1.57	1.02
1:A:306:GLN:HG2	4:A:2074:HOH:O	1.58	1.01
1:A:429:GLU:HB3	4:A:2244:HOH:O	1.62	0.99
1:A:377:ALA:HB3	4:A:2203:HOH:O	1.63	0.97
2:B:515:ARG:HA	4:B:2250:HOH:O	1.63	0.97
1:A:414:GLU:HB3	4:A:2238:HOH:O	1.63	0.97
1:A:263:SER:HB2	4:A:2023:HOH:O	1.63	0.97
1:A:257:LYS:HD3	4:A:2022:HOH:O	1.62	0.96
2:B:317:LYS:HD3	4:B:2081:HOH:O	1.64	0.96
2:B:398:ALA:HB2	4:B:2179:HOH:O	1.66	0.95
1:A:420:SER:HB3	4:A:2241:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:HD3	4:A:2124:HOH:O	1.67	0.95
1:A:325:ILE:HB	4:A:2095:HOH:O	1.65	0.95
2:B:226:ASP:HA	2:B:229:THR:HG22	1.47	0.95
2:B:244:ALA:HB2	4:B:2015:HOH:O	1.69	0.93
1:A:345:GLU:HB3	4:A:2152:HOH:O	1.67	0.93
2:B:265:ARG:HG2	4:B:2036:HOH:O	1.69	0.93
1:A:412:ILE:HD11	4:B:2106:HOH:O	1.68	0.92
1:A:454:MET:HG2	4:B:2059:HOH:O	1.68	0.92
2:B:413:ALA:HB3	4:B:2194:HOH:O	1.69	0.91
2:B:497:LEU:HD13	4:B:2026:HOH:O	1.71	0.89
1:A:490:VAL:HG11	4:A:2023:HOH:O	1.73	0.88
1:A:447:ALA:HA	4:B:2065:HOH:O	1.73	0.88
4:A:2056:HOH:O	2:B:454:MET:HE3	1.71	0.88
1:A:475:ALA:HA	4:A:2278:HOH:O	1.74	0.87
2:B:406:VAL:HG23	4:B:2185:HOH:O	1.72	0.87
1:A:427:VAL:HG22	4:A:2095:HOH:O	1.75	0.87
2:B:299:SER:HB3	4:B:2062:HOH:O	1.74	0.86
2:B:316:LYS:HA	4:B:2080:HOH:O	1.74	0.86
2:B:402:VAL:HG13	4:B:2185:HOH:O	1.74	0.86
1:A:224:MET:HB3	4:A:2001:HOH:O	1.76	0.85
2:B:481:LYS:HE3	4:B:2230:HOH:O	1.74	0.85
2:B:310:GLU:HA	2:B:313:ASP:HB2	1.57	0.85
2:B:294:ALA:HB2	2:B:458:ILE:HD11	1.56	0.85
1:A:225:LYS:HD3	4:A:2001:HOH:O	1.78	0.84
1:A:366:ASN:HB3	4:A:2184:HOH:O	1.78	0.83
2:B:253:LEU:HD12	4:B:2027:HOH:O	1.76	0.83
2:B:322:THR:HG23	2:B:427:VAL:HG22	1.60	0.83
2:B:270:SER:HB2	4:B:2039:HOH:O	1.79	0.83
1:A:350:VAL:HG12	4:A:2162:HOH:O	1.78	0.83
4:A:2219:HOH:O	2:B:236:GLU:HG2	1.79	0.83
2:B:355:ALA:HB1	4:B:2139:HOH:O	1.77	0.83
1:A:354:ASN:HB3	4:A:2164:HOH:O	1.78	0.83
2:B:515:ARG:HG3	4:B:2250:HOH:O	1.79	0.83
1:A:342:GLY:HA2	4:A:2152:HOH:O	1.78	0.82
2:B:316:LYS:HG3	4:B:2079:HOH:O	1.78	0.82
2:B:367:ALA:HB1	4:B:2147:HOH:O	1.79	0.81
2:B:526:ALA:HB2	4:B:2256:HOH:O	1.80	0.81
4:A:2040:HOH:O	2:B:468:ALA:HB1	1.79	0.81
1:A:228:GLN:HG3	1:A:525:VAL:HG21	1.64	0.79
1:A:454:MET:CG	4:B:2059:HOH:O	2.26	0.79
1:A:433:LEU:HB3	4:A:2250:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:HB3	4:B:2036:HOH:O	1.82	0.79
2:B:500:ILE:HG13	4:B:2242:HOH:O	1.82	0.79
1:A:369:ILE:HD13	4:A:2154:HOH:O	1.82	0.79
2:B:522:LYS:CG	4:B:2061:HOH:O	2.30	0.78
1:A:500:ILE:HG22	4:A:2297:HOH:O	1.83	0.78
2:B:225:LYS:CB	4:B:2002:HOH:O	2.30	0.78
2:B:507:VAL:CG2	4:B:2016:HOH:O	2.31	0.78
2:B:522:LYS:HG3	4:B:2061:HOH:O	1.84	0.78
1:A:317:LYS:HG3	4:A:2081:HOH:O	1.85	0.77
1:A:369:ILE:CD1	4:A:2154:HOH:O	2.31	0.77
1:A:402:VAL:HG23	2:B:346:ILE:CD1	2.15	0.77
2:B:244:ALA:O	2:B:248:ILE:HG12	1.85	0.77
1:A:475:ALA:CA	4:A:2278:HOH:O	2.30	0.77
2:B:316:LYS:CA	4:B:2080:HOH:O	2.31	0.76
1:A:252:LEU:HD21	4:A:2297:HOH:O	1.85	0.76
2:B:270:SER:CB	4:B:2039:HOH:O	2.34	0.75
2:B:350:VAL:HA	4:B:2131:HOH:O	1.86	0.75
1:A:353:ILE:HD11	2:B:398:ALA:HB3	1.68	0.75
1:A:402:VAL:HG23	2:B:346:ILE:HD11	1.69	0.74
1:A:503:SER:HB2	2:B:248:ILE:HD11	1.70	0.73
2:B:522:LYS:HB2	4:B:2061:HOH:O	1.87	0.73
1:A:332:VAL:CG2	4:A:2109:HOH:O	2.36	0.73
2:B:440:LYS:NZ	4:B:2206:HOH:O	2.20	0.73
2:B:267:GLU:HG2	4:B:2038:HOH:O	1.89	0.72
1:A:227:VAL:HG22	4:A:2006:HOH:O	1.89	0.72
2:B:481:LYS:CE	4:B:2229:HOH:O	2.37	0.72
2:B:244:ALA:CA	4:B:2015:HOH:O	2.37	0.72
2:B:223:HIS:C	2:B:225:LYS:H	1.90	0.72
1:A:346:ILE:HG13	4:A:2152:HOH:O	1.89	0.72
1:A:354:ASN:CB	4:A:2164:HOH:O	2.33	0.72
1:A:363:LEU:HD21	2:B:387:GLU:HG3	1.71	0.72
2:B:420:SER:HB2	4:B:2200:HOH:O	1.88	0.72
1:A:353:ILE:HD11	2:B:398:ALA:CB	2.20	0.72
1:A:273:VAL:HG22	1:A:476:MET:HE3	1.71	0.71
1:A:377:ALA:CA	4:A:2203:HOH:O	2.37	0.71
1:A:485:GLU:CB	4:B:2036:HOH:O	2.36	0.70
2:B:396:GLN:HG2	2:B:397:GLN:HE21	1.56	0.70
1:A:235:ALA:C	4:A:2008:HOH:O	2.29	0.70
1:A:268:SER:HB3	4:A:2033:HOH:O	1.91	0.70
2:B:228:GLN:HA	2:B:231:THR:HG22	1.72	0.70
2:B:297:ALA:N	4:B:2059:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ALA:C	4:A:2183:HOH:O	2.30	0.70
1:A:399:SER:HA	1:A:402:VAL:HG12	1.74	0.70
1:A:295:GLN:NE2	4:A:2055:HOH:O	2.25	0.70
2:B:504:THR:HA	4:B:2016:HOH:O	1.90	0.69
2:B:369:ILE:HG13	4:B:2146:HOH:O	1.91	0.69
1:A:475:ALA:CB	4:A:2278:HOH:O	2.40	0.69
1:A:351:GLU:N	4:A:2162:HOH:O	2.25	0.69
2:B:329:ALA:HB2	2:B:423:ILE:HG21	1.75	0.69
1:A:268:SER:CB	4:A:2033:HOH:O	2.41	0.69
2:B:512:GLN:HG2	4:B:2251:HOH:O	1.92	0.68
1:A:331:ASP:HB2	2:B:419:VAL:HG11	1.74	0.68
2:B:351:GLU:HB3	4:B:2119:HOH:O	1.92	0.68
1:A:510:ARG:NE	4:A:2303:HOH:O	2.26	0.68
2:B:265:ARG:NE	4:B:2036:HOH:O	2.25	0.68
1:A:454:MET:SD	4:B:2059:HOH:O	2.50	0.68
1:A:329:ALA:HA	4:A:2109:HOH:O	1.92	0.68
2:B:414:GLU:N	4:B:2194:HOH:O	2.27	0.68
2:B:238:ILE:HD11	2:B:511:VAL:O	1.93	0.68
1:A:317:LYS:CG	4:A:2081:HOH:O	2.41	0.68
2:B:515:ARG:CA	4:B:2250:HOH:O	2.31	0.67
1:A:344:GLU:O	1:A:348:SER:HB2	1.94	0.67
1:A:297:ALA:N	4:A:2063:HOH:O	2.27	0.67
2:B:351:GLU:HG2	4:B:2133:HOH:O	1.94	0.67
2:B:379:ARG:NH2	4:B:2157:HOH:O	2.27	0.67
2:B:244:ALA:CB	4:B:2015:HOH:O	2.34	0.67
2:B:316:LYS:HD2	4:B:2080:HOH:O	1.93	0.67
2:B:265:ARG:CG	4:B:2036:HOH:O	2.34	0.67
2:B:497:LEU:HD22	4:B:2026:HOH:O	1.94	0.67
2:B:481:LYS:HE2	4:B:2229:HOH:O	1.95	0.67
1:A:368:ALA:HB2	4:A:2183:HOH:O	1.93	0.67
2:B:311:ALA:HB1	2:B:441:LEU:HD21	1.77	0.67
1:A:442:ASN:ND2	4:A:2257:HOH:O	2.27	0.67
2:B:420:SER:CB	4:B:2200:HOH:O	2.42	0.67
2:B:466:ASN:ND2	4:B:2220:HOH:O	2.27	0.67
1:A:408:GLU:O	1:A:412:ILE:HG12	1.96	0.66
2:B:418:LYS:HG3	2:B:422:GLU:HB2	1.77	0.66
1:A:491:LYS:NZ	4:A:2288:HOH:O	2.28	0.66
2:B:317:LYS:HA	4:B:2081:HOH:O	1.95	0.66
1:A:342:GLY:CA	4:A:2152:HOH:O	2.40	0.66
1:A:223:HIS:CE1	4:A:2002:HOH:O	2.47	0.66
1:A:428:GLU:HA	1:A:431:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ARG:NH1	4:B:2034:HOH:O	2.28	0.66
1:A:475:ALA:HB2	4:A:2278:HOH:O	1.95	0.66
2:B:238:ILE:CD1	4:B:2250:HOH:O	2.43	0.65
1:A:378:GLY:N	4:A:2203:HOH:O	2.29	0.65
1:A:462:ILE:N	4:A:2270:HOH:O	2.29	0.65
1:A:522:LYS:O	1:A:525:VAL:HG12	1.97	0.65
2:B:316:LYS:N	4:B:2080:HOH:O	2.27	0.65
1:A:252:LEU:CD2	4:A:2297:HOH:O	2.42	0.65
1:A:420:SER:CB	4:A:2241:HOH:O	2.35	0.64
1:A:227:VAL:CG2	4:A:2006:HOH:O	2.45	0.64
2:B:315:LEU:C	4:B:2080:HOH:O	2.35	0.64
1:A:347:THR:O	1:A:351:GLU:HG2	1.96	0.64
1:A:282:GLU:CD	4:A:2044:HOH:O	2.36	0.64
2:B:398:ALA:N	4:B:2179:HOH:O	2.31	0.64
2:B:284:SER:O	2:B:287:THR:HG22	1.98	0.63
1:A:505:GLU:HG3	4:A:2298:HOH:O	1.98	0.63
2:B:330:LYS:HA	4:B:2095:HOH:O	1.97	0.63
1:A:377:ALA:N	4:A:2203:HOH:O	2.31	0.63
1:A:488:ASN:ND2	4:A:2287:HOH:O	2.31	0.63
4:A:2180:HOH:O	2:B:360:THR:HG21	1.98	0.63
2:B:279:GLY:O	2:B:283:ILE:HG12	1.98	0.63
1:A:451:ILE:CD1	4:B:2068:HOH:O	2.47	0.63
2:B:439:GLU:HA	2:B:442:ASN:OD1	1.98	0.63
2:B:238:ILE:HD12	4:B:2250:HOH:O	1.98	0.63
1:A:416:ALA:HA	4:A:2239:HOH:O	1.98	0.63
2:B:410:ARG:NH1	4:B:2192:HOH:O	2.30	0.63
1:A:503:SER:HB2	2:B:248:ILE:CD1	2.29	0.62
1:A:515:ARG:HB2	4:A:2009:HOH:O	1.98	0.62
1:A:385:ALA:HB1	4:A:2183:HOH:O	1.99	0.62
1:A:355:ALA:N	4:A:2170:HOH:O	2.31	0.62
1:A:496:ARG:N	1:A:496:ARG:HD2	2.15	0.61
1:A:507:VAL:HG13	2:B:241:ILE:HG13	1.82	0.61
1:A:259:MET:CE	1:A:493:VAL:HG11	2.29	0.61
1:A:527:ARG:HG3	1:A:528:TYR:CD1	2.35	0.61
1:A:432:LYS:HE3	4:A:2253:HOH:O	2.00	0.61
2:B:243:LYS:HG2	4:B:2020:HOH:O	1.99	0.61
2:B:497:LEU:CD1	4:B:2026:HOH:O	2.38	0.61
1:A:237:SER:CB	2:B:514:ILE:HD11	2.30	0.61
1:A:377:ALA:CB	4:A:2203:HOH:O	2.30	0.61
1:A:369:ILE:CG2	4:A:2185:HOH:O	2.47	0.61
1:A:244:ALA:HB2	2:B:506:GLU:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:ASN:ND2	4:B:2144:HOH:O	2.33	0.60
1:A:416:ALA:O	1:A:419:VAL:HG22	2.01	0.60
1:A:354:ASN:C	4:A:2170:HOH:O	2.39	0.60
1:A:332:VAL:HG23	4:A:2109:HOH:O	1.98	0.60
2:B:301:ALA:C	4:B:2063:HOH:O	2.39	0.60
1:A:433:LEU:HD22	4:A:2250:HOH:O	2.00	0.60
1:A:471:GLU:HB2	4:B:2047:HOH:O	2.02	0.60
1:A:257:LYS:NZ	4:A:2022:HOH:O	2.34	0.60
1:A:317:LYS:CD	4:A:2081:HOH:O	2.50	0.59
2:B:510:ARG:O	2:B:514:ILE:HD13	2.03	0.59
1:A:451:ILE:HD12	4:B:2068:HOH:O	2.02	0.59
2:B:495:ALA:HA	4:B:2238:HOH:O	2.02	0.59
1:A:412:ILE:HD12	2:B:334:ARG:NH1	2.17	0.59
2:B:226:ASP:HA	2:B:229:THR:CG2	2.28	0.59
1:A:433:LEU:CB	4:A:2250:HOH:O	2.46	0.59
2:B:507:VAL:HG21	4:B:2016:HOH:O	1.97	0.59
1:A:522:LYS:HG2	4:A:2313:HOH:O	2.02	0.59
1:A:326:SER:HB2	4:A:2102:HOH:O	2.02	0.59
2:B:408:GLU:O	2:B:412:ILE:HG12	2.03	0.59
2:B:452:ASN:ND2	4:B:2212:HOH:O	2.36	0.59
2:B:267:GLU:HG2	4:B:2037:HOH:O	2.01	0.59
1:A:343:ALA:O	1:A:347:THR:HB	2.03	0.58
1:A:313:ASP:O	1:A:317:LYS:HD3	2.03	0.58
1:A:363:LEU:HD23	2:B:388:ILE:HG13	1.85	0.58
2:B:329:ALA:CB	2:B:423:ILE:HG21	2.33	0.58
2:B:466:ASN:HA	4:B:2220:HOH:O	2.02	0.58
1:A:422:GLU:HG3	4:A:2242:HOH:O	2.03	0.58
2:B:434:ALA:N	4:B:2203:HOH:O	2.35	0.58
1:A:296:GLN:C	4:A:2063:HOH:O	2.41	0.58
2:B:223:HIS:ND1	4:B:2002:HOH:O	2.32	0.58
2:B:410:ARG:HH11	2:B:410:ARG:HG3	1.69	0.58
1:A:289:ASN:ND2	4:A:2050:HOH:O	2.36	0.58
1:A:318:VAL:CG1	4:B:2203:HOH:O	2.28	0.58
2:B:378:GLY:N	4:B:2156:HOH:O	2.36	0.58
2:B:346:ILE:CB	4:B:2120:HOH:O	2.31	0.58
1:A:525:VAL:N	4:A:2312:HOH:O	2.36	0.58
1:A:248:ILE:HD13	4:B:2242:HOH:O	2.04	0.58
1:A:321:VAL:O	1:A:325:ILE:HG12	2.04	0.58
1:A:417:GLY:CA	4:A:2116:HOH:O	2.52	0.58
1:A:417:GLY:HA3	4:A:2116:HOH:O	2.03	0.58
2:B:398:ALA:CA	4:B:2179:HOH:O	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG13	2:B:255:ILE:HD12	1.84	0.57
1:A:332:VAL:O	1:A:336:VAL:HG23	2.04	0.57
1:A:436:GLU:O	1:A:440:LYS:HG2	2.04	0.57
1:A:522:LYS:CD	4:A:2313:HOH:O	2.51	0.57
2:B:222:SER:N	4:B:2001:HOH:O	2.37	0.57
1:A:433:LEU:HD21	2:B:317:LYS:HB3	1.85	0.57
2:B:275:GLU:CG	4:B:2047:HOH:O	2.51	0.57
2:B:526:ALA:CB	4:B:2260:HOH:O	2.33	0.57
1:A:429:GLU:N	4:A:2244:HOH:O	2.37	0.57
2:B:522:LYS:CB	4:B:2061:HOH:O	2.44	0.57
1:A:507:VAL:O	1:A:511:VAL:HG23	2.04	0.57
1:A:426:ARG:NH1	4:A:2246:HOH:O	2.36	0.57
1:A:462:ILE:HG13	4:A:2270:HOH:O	2.04	0.57
1:A:339:PHE:CE1	2:B:409:ILE:HG23	2.40	0.57
1:A:356:ILE:HG22	4:A:2171:HOH:O	2.05	0.57
1:A:399:SER:HA	1:A:402:VAL:CG1	2.35	0.57
1:A:325:ILE:HD11	2:B:426:ARG:HB3	1.85	0.57
2:B:441:LEU:HD12	2:B:444:ILE:HG21	1.86	0.57
1:A:267:GLU:HA	4:A:2029:HOH:O	2.03	0.57
1:A:394:GLU:HG3	4:A:2167:HOH:O	2.05	0.56
2:B:346:ILE:CA	4:B:2120:HOH:O	2.53	0.56
2:B:273:VAL:HG22	2:B:476:MET:HE3	1.87	0.56
2:B:364:ALA:HB3	4:B:2143:HOH:O	2.05	0.56
1:A:318:VAL:HG12	2:B:433:LEU:HB2	1.85	0.56
2:B:255:ILE:HB	4:B:2026:HOH:O	2.03	0.56
2:B:398:ALA:O	2:B:402:VAL:HG23	2.06	0.56
1:A:523:GLU:HB2	4:A:2311:HOH:O	2.05	0.56
2:B:321:VAL:O	2:B:325:ILE:HG22	2.06	0.55
1:A:334:ARG:CD	4:A:2124:HOH:O	2.38	0.55
1:A:366:ASN:ND2	4:A:2185:HOH:O	2.38	0.55
1:A:339:PHE:HE1	2:B:409:ILE:HG23	1.71	0.55
1:A:385:ALA:CB	4:A:2183:HOH:O	2.53	0.55
1:A:462:ILE:CA	4:A:2270:HOH:O	2.55	0.55
2:B:346:ILE:N	4:B:2120:HOH:O	2.39	0.55
2:B:423:ILE:HG22	2:B:424:THR:N	2.20	0.55
2:B:517:ASN:ND2	4:B:2254:HOH:O	2.33	0.55
2:B:330:LYS:CA	4:B:2095:HOH:O	2.55	0.55
2:B:515:ARG:O	2:B:518:VAL:HG12	2.07	0.55
1:A:498:GLN:HG2	4:A:2295:HOH:O	2.06	0.55
1:A:315:LEU:O	1:A:318:VAL:HG22	2.07	0.55
2:B:248:ILE:HG21	4:B:2242:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:GLN:HG3	4:B:2177:HOH:O	2.07	0.54
2:B:238:ILE:HD13	2:B:515:ARG:HG3	1.90	0.54
1:A:528:TYR:OH	2:B:223:HIS:HB2	2.07	0.54
2:B:484:GLU:HG2	4:B:2231:HOH:O	2.05	0.54
2:B:507:VAL:HB	4:B:2016:HOH:O	2.08	0.54
1:A:237:SER:HB2	2:B:514:ILE:HD11	1.90	0.54
2:B:326:SER:HB2	4:B:2089:HOH:O	2.07	0.54
1:A:517:ASN:OD1	2:B:233:SER:HB3	2.08	0.54
2:B:343:ALA:O	2:B:346:ILE:HG22	2.08	0.53
1:A:522:LYS:HD2	4:A:2313:HOH:O	2.07	0.53
1:A:305:THR:O	1:A:309:LYS:HG2	2.08	0.53
2:B:434:ALA:CA	4:B:2203:HOH:O	2.56	0.53
2:B:255:ILE:O	2:B:259:MET:HB2	2.09	0.53
2:B:434:ALA:HA	4:B:2203:HOH:O	2.08	0.53
2:B:455:LEU:CD2	4:B:2212:HOH:O	2.56	0.53
1:A:404:ARG:HG3	4:A:2234:HOH:O	2.09	0.53
1:A:251:GLN:HG3	4:A:2020:HOH:O	2.08	0.53
2:B:526:ALA:CA	4:B:2260:HOH:O	2.55	0.53
2:B:402:VAL:CG1	4:B:2185:HOH:O	2.41	0.53
2:B:507:VAL:O	2:B:511:VAL:HG23	2.08	0.52
1:A:283:ILE:O	1:A:287:THR:HG23	2.08	0.52
4:A:2040:HOH:O	2:B:468:ALA:CB	2.49	0.52
1:A:227:VAL:HA	4:A:2006:HOH:O	2.09	0.52
2:B:223:HIS:C	2:B:225:LYS:N	2.63	0.52
1:A:248:ILE:CD1	4:B:2242:HOH:O	2.57	0.52
1:A:331:ASP:HB2	2:B:419:VAL:CG1	2.40	0.52
4:A:2020:HOH:O	2:B:496:ARG:CD	2.28	0.52
1:A:426:ARG:HA	1:A:429:GLU:HG2	1.91	0.52
1:A:366:ASN:O	1:A:370:GLU:HB2	2.10	0.52
1:A:248:ILE:HG23	2:B:500:ILE:HD12	1.91	0.52
2:B:527:ARG:NH2	4:B:2263:HOH:O	2.36	0.52
4:A:2142:HOH:O	2:B:412:ILE:HD11	2.09	0.52
1:A:258:GLU:HG3	2:B:489:SER:HB3	1.92	0.52
1:A:330:LYS:CA	4:A:2112:HOH:O	2.36	0.51
1:A:237:SER:HB3	2:B:514:ILE:HD11	1.92	0.51
1:A:462:ILE:HA	4:A:2270:HOH:O	2.10	0.51
2:B:405:VAL:HG23	4:B:2185:HOH:O	2.10	0.51
2:B:524:ILE:CD1	2:B:527:ARG:HH11	2.23	0.51
2:B:317:LYS:CD	4:B:2081:HOH:O	2.39	0.51
2:B:226:ASP:O	2:B:230:GLU:HB2	2.10	0.51
1:A:404:ARG:O	1:A:408:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:GLU:HG2	4:B:2172:HOH:O	2.09	0.51
1:A:369:ILE:HG21	4:A:2185:HOH:O	2.10	0.51
1:A:223:HIS:HE1	4:A:2002:HOH:O	1.88	0.51
2:B:381:PHE:HA	2:B:384:VAL:HG22	1.93	0.51
2:B:470:ASP:O	2:B:474:THR:HG22	2.11	0.51
2:B:433:LEU:C	4:B:2203:HOH:O	2.48	0.51
2:B:455:LEU:HD23	4:B:2212:HOH:O	2.11	0.51
2:B:320:GLU:HA	2:B:323:ARG:HG3	1.93	0.51
2:B:246:GLU:HA	2:B:249:THR:HG22	1.91	0.50
2:B:350:VAL:CA	4:B:2131:HOH:O	2.53	0.50
1:A:257:LYS:CD	4:A:2022:HOH:O	2.39	0.50
2:B:416:ALA:O	2:B:419:VAL:HG22	2.11	0.50
1:A:501:SER:HA	4:A:2297:HOH:O	2.11	0.50
1:A:259:MET:HE3	1:A:493:VAL:HG11	1.92	0.50
1:A:463:GLU:O	1:A:466:THR:HG22	2.11	0.50
2:B:235:ALA:HB2	2:B:518:VAL:HG21	1.94	0.50
2:B:247:GLU:HB3	4:B:2019:HOH:O	2.10	0.50
2:B:246:GLU:O	2:B:249:THR:HG22	2.12	0.50
2:B:317:LYS:CA	4:B:2081:HOH:O	2.56	0.50
1:A:240:GLU:HA	1:A:243:LYS:HE2	1.93	0.50
2:B:248:ILE:CG2	2:B:500:ILE:HD11	2.42	0.50
1:A:235:ALA:CB	4:A:2008:HOH:O	2.60	0.50
2:B:295:GLN:O	2:B:298:ALA:HB3	2.12	0.49
1:A:349:PHE:O	1:A:353:ILE:HG12	2.12	0.49
1:A:390:LYS:CA	4:A:2215:HOH:O	2.27	0.49
1:A:402:VAL:CG2	2:B:346:ILE:HD11	2.41	0.49
2:B:414:GLU:HG2	4:B:2194:HOH:O	2.13	0.49
2:B:287:THR:HG21	4:B:2220:HOH:O	2.11	0.49
2:B:275:GLU:CD	4:B:2047:HOH:O	2.50	0.49
1:A:365:LEU:HG	1:A:389:ARG:HD3	1.95	0.49
2:B:482:ASN:N	4:B:2230:HOH:O	2.45	0.49
2:B:401:ASN:HD22	2:B:401:ASN:N	2.09	0.49
1:A:271:ALA:HB2	4:A:2032:HOH:O	2.13	0.49
1:A:453:GLU:HG2	4:A:2268:HOH:O	2.12	0.49
1:A:234:VAL:HG12	2:B:517:ASN:HB3	1.95	0.49
1:A:273:VAL:HA	1:A:476:MET:HE3	1.95	0.49
2:B:322:THR:HG23	2:B:427:VAL:CG2	2.35	0.49
1:A:522:LYS:CG	4:A:2313:HOH:O	2.60	0.49
1:A:528:TYR:CE2	2:B:223:HIS:HB3	2.48	0.49
1:A:451:ILE:HD11	4:B:2068:HOH:O	2.11	0.49
1:A:261:ASN:HB3	1:A:265:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:HD12	2:B:334:ARG:HH12	1.78	0.48
1:A:251:GLN:NE2	4:A:2020:HOH:O	2.20	0.48
1:A:515:ARG:CB	4:A:2009:HOH:O	2.58	0.48
1:A:450:ARG:HD3	2:B:300:PHE:CE2	2.49	0.48
2:B:273:VAL:HG13	2:B:476:MET:HG3	1.94	0.48
1:A:272:SER:HA	1:A:275:GLU:OE2	2.14	0.48
1:A:235:ALA:HB2	1:A:518:VAL:HG21	1.96	0.48
2:B:317:LYS:CG	4:B:2081:HOH:O	2.59	0.48
1:A:350:VAL:C	4:A:2162:HOH:O	2.49	0.48
1:A:395:SER:OG	2:B:356:ILE:HG21	2.13	0.48
2:B:257:LYS:HD3	4:B:2028:HOH:O	2.12	0.48
2:B:468:ALA:O	2:B:472:ILE:HG13	2.13	0.48
2:B:497:LEU:CD2	4:B:2026:HOH:O	2.56	0.48
2:B:375:GLY:C	2:B:377:ALA:H	2.16	0.48
2:B:484:GLU:CG	4:B:2231:HOH:O	2.62	0.48
2:B:243:LYS:NZ	4:B:2007:HOH:O	2.45	0.48
1:A:235:ALA:HB2	1:A:518:VAL:CG2	2.44	0.48
2:B:297:ALA:CA	4:B:2059:HOH:O	2.62	0.47
2:B:390:LYS:CB	4:B:2163:HOH:O	2.62	0.47
2:B:347:THR:O	2:B:350:VAL:HB	2.14	0.47
1:A:278:ALA:O	1:A:282:GLU:HG3	2.13	0.47
1:A:485:GLU:HB2	4:B:2036:HOH:O	2.07	0.47
2:B:445:VAL:O	2:B:449:GLU:HB2	2.15	0.47
2:B:405:VAL:CG2	4:B:2185:HOH:O	2.62	0.47
2:B:381:PHE:N	2:B:381:PHE:CD2	2.80	0.47
2:B:323:ARG:NH2	4:B:2090:HOH:O	2.47	0.47
1:A:337:GLU:HA	1:A:340:GLN:HB3	1.97	0.47
1:A:409:ILE:HG13	4:B:2114:HOH:O	2.15	0.47
2:B:507:VAL:HG21	4:B:2017:HOH:O	2.14	0.47
1:A:379:ARG:HD3	4:A:2205:HOH:O	2.13	0.47
2:B:423:ILE:HD13	2:B:423:ILE:HA	1.73	0.47
1:A:431:THR:HG23	1:A:432:LYS:N	2.30	0.47
1:A:517:ASN:O	1:A:521:LEU:HG	2.14	0.47
1:A:440:LYS:HD2	2:B:307:LEU:HD22	1.97	0.47
1:A:319:ILE:HG21	4:A:2255:HOH:O	2.14	0.47
2:B:526:ALA:C	4:B:2260:HOH:O	2.53	0.47
2:B:223:HIS:CE1	4:B:2002:HOH:O	2.68	0.46
2:B:238:ILE:HD13	4:B:2250:HOH:O	2.12	0.46
1:A:319:ILE:HG12	1:A:319:ILE:H	1.54	0.46
2:B:389:ARG:HA	4:B:2143:HOH:O	2.15	0.46
2:B:441:LEU:O	2:B:444:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:ALA:O	2:B:428:GLU:HB3	2.16	0.46
1:A:390:LYS:C	4:A:2212:HOH:O	2.53	0.46
2:B:244:ALA:HA	4:B:2015:HOH:O	2.11	0.46
2:B:497:LEU:O	2:B:500:ILE:HG23	2.16	0.46
2:B:504:THR:HG22	4:B:2244:HOH:O	2.15	0.46
2:B:303:GLN:NE2	4:B:2065:HOH:O	2.49	0.45
2:B:487:THR:HG23	4:B:2032:HOH:O	2.17	0.45
2:B:437:ALA:O	2:B:441:LEU:HB2	2.17	0.45
2:B:409:ILE:O	2:B:412:ILE:HB	2.16	0.45
1:A:515:ARG:HD3	4:A:2009:HOH:O	2.15	0.45
1:A:329:ALA:HB1	1:A:423:ILE:HD12	1.99	0.45
1:A:327:ASN:O	1:A:330:LYS:HB3	2.17	0.45
2:B:265:ARG:O	2:B:269:ILE:HG12	2.17	0.45
1:A:318:VAL:HG12	2:B:433:LEU:CB	2.47	0.45
2:B:481:LYS:CE	4:B:2230:HOH:O	2.48	0.45
1:A:243:LYS:NZ	4:A:2016:HOH:O	2.47	0.45
1:A:283:ILE:HD11	2:B:468:ALA:HB3	1.99	0.44
1:A:511:VAL:HG11	4:A:2014:HOH:O	2.17	0.44
1:A:303:GLN:O	1:A:307:LEU:HG	2.16	0.44
2:B:424:THR:HA	2:B:427:VAL:HG12	1.98	0.44
2:B:441:LEU:HD12	2:B:444:ILE:CG2	2.46	0.44
1:A:441:LEU:O	1:A:444:ILE:HG12	2.17	0.44
1:A:266:ILE:HD13	1:A:266:ILE:HA	1.81	0.44
1:A:358:GLU:CG	4:A:2178:HOH:O	2.65	0.44
2:B:294:ALA:CB	2:B:458:ILE:HD11	2.37	0.44
1:A:323:ARG:HD3	4:A:2102:HOH:O	2.16	0.44
2:B:419:VAL:O	2:B:423:ILE:HG12	2.17	0.44
2:B:230:GLU:O	2:B:234:VAL:HG13	2.18	0.44
1:A:516:GLU:HG3	1:A:517:ASN:N	2.33	0.44
1:A:441:LEU:O	1:A:445:VAL:HG23	2.17	0.44
2:B:481:LYS:C	4:B:2230:HOH:O	2.55	0.44
1:A:295:GLN:HG2	4:A:2055:HOH:O	2.18	0.44
1:A:447:ALA:CB	4:B:2065:HOH:O	2.65	0.44
1:A:243:LYS:CE	4:A:2016:HOH:O	2.65	0.44
4:A:2003:HOH:O	2:B:224:MET:HG3	2.18	0.44
2:B:505:GLU:O	2:B:508:THR:HG22	2.18	0.44
1:A:273:VAL:HG13	1:A:476:MET:HG3	1.99	0.43
1:A:454:MET:HG2	2:B:293:SER:O	2.17	0.43
2:B:322:THR:HG21	2:B:431:THR:OG1	2.18	0.43
2:B:288:LYS:NZ	4:B:2054:HOH:O	2.39	0.43
1:A:250:ASN:ND2	4:A:2019:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:SER:O	1:A:415:ASP:HB2	2.19	0.43
1:A:496:ARG:CB	2:B:255:ILE:HD11	2.49	0.43
1:A:359:GLN:O	1:A:363:LEU:HB2	2.18	0.43
2:B:243:LYS:HD3	4:B:2007:HOH:O	2.19	0.43
2:B:390:LYS:HB2	4:B:2163:HOH:O	2.18	0.43
2:B:252:LEU:HD11	2:B:500:ILE:HD13	2.01	0.43
1:A:243:LYS:HE3	4:A:2016:HOH:O	2.19	0.43
1:A:273:VAL:HA	1:A:476:MET:CE	2.49	0.43
2:B:473:THR:HA	4:B:2225:HOH:O	2.19	0.43
2:B:261:ASN:N	2:B:261:ASN:HD22	2.17	0.42
1:A:496:ARG:HB2	2:B:255:ILE:HD11	2.01	0.42
2:B:481:LYS:HB3	4:B:2230:HOH:O	2.19	0.42
1:A:332:VAL:HG21	4:A:2109:HOH:O	2.11	0.42
2:B:315:LEU:C	2:B:317:LYS:H	2.23	0.42
1:A:315:LEU:HD21	2:B:315:LEU:HD21	2.01	0.42
1:A:323:ARG:HD3	1:A:323:ARG:HA	1.72	0.42
2:B:310:GLU:CA	2:B:313:ASP:HB2	2.40	0.42
1:A:233:SER:HB3	2:B:517:ASN:OD1	2.20	0.42
2:B:500:ILE:CG1	4:B:2242:HOH:O	2.53	0.42
2:B:384:VAL:HG23	2:B:385:ALA:N	2.35	0.42
2:B:287:THR:HG21	2:B:466:ASN:ND2	2.35	0.42
1:A:323:ARG:NH2	4:A:2097:HOH:O	2.28	0.42
2:B:227:VAL:CG1	2:B:228:GLN:N	2.82	0.42
1:A:452:ASN:O	1:A:456:GLN:HG3	2.20	0.42
1:A:399:SER:CA	1:A:402:VAL:HG12	2.48	0.42
1:A:369:ILE:HD11	4:A:2154:HOH:O	2.12	0.42
1:A:466:THR:O	1:A:469:VAL:HG12	2.20	0.42
1:A:376:GLU:O	1:A:379:ARG:HB2	2.20	0.42
1:A:279:GLY:CA	4:A:2040:HOH:O	2.30	0.42
2:B:398:ALA:CB	4:B:2179:HOH:O	2.38	0.42
1:A:523:GLU:HG3	4:A:2311:HOH:O	2.20	0.42
1:A:428:GLU:CA	1:A:431:THR:HG22	2.49	0.41
1:A:417:GLY:HA2	4:A:2116:HOH:O	2.19	0.41
1:A:451:ILE:O	1:A:455:LEU:HD22	2.20	0.41
2:B:396:GLN:HG2	2:B:397:GLN:N	2.34	0.41
1:A:306:GLN:O	1:A:310:GLU:HB2	2.20	0.41
1:A:510:ARG:HD3	1:A:510:ARG:HA	1.94	0.41
1:A:325:ILE:CG2	4:A:2095:HOH:O	2.68	0.41
2:B:303:GLN:O	2:B:307:LEU:HG	2.20	0.41
2:B:473:THR:HA	4:B:2224:HOH:O	2.19	0.41
1:A:288:LYS:HD3	4:A:2091:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:N	4:A:2215:HOH:O	2.47	0.41
1:A:263:SER:CB	4:A:2023:HOH:O	2.42	0.41
1:A:379:ARG:CD	4:A:2205:HOH:O	2.69	0.41
1:A:389:ARG:NH2	4:A:2215:HOH:O	2.54	0.41
2:B:231:THR:HA	2:B:234:VAL:HG22	2.03	0.41
1:A:369:ILE:HD11	4:A:2140:HOH:O	2.20	0.41
1:A:339:PHE:CE1	2:B:339:PHE:HB3	2.55	0.41
2:B:244:ALA:N	4:B:2015:HOH:O	2.51	0.41
1:A:290:ILE:HG22	1:A:462:ILE:HD11	2.03	0.41
1:A:402:VAL:HG23	2:B:346:ILE:HD12	2.00	0.41
1:A:325:ILE:CB	4:A:2095:HOH:O	2.44	0.41
2:B:299:SER:O	2:B:302:ASP:HB2	2.21	0.41
1:A:523:GLU:CB	4:A:2311:HOH:O	2.65	0.41
1:A:250:ASN:ND2	4:A:2018:HOH:O	2.53	0.41
1:A:514:ILE:HD11	2:B:237:SER:HB2	2.02	0.41
1:A:447:ALA:CA	4:B:2065:HOH:O	2.47	0.41
1:A:224:MET:HG2	1:A:529:LYS:CB	2.51	0.41
1:A:255:ILE:HG22	1:A:497:LEU:HD11	2.03	0.41
2:B:496:ARG:O	2:B:500:ILE:HG22	2.21	0.40
1:A:330:LYS:C	4:A:2112:HOH:O	2.58	0.40
1:A:363:LEU:HD23	2:B:388:ILE:CG1	2.51	0.40
1:A:428:GLU:HA	1:A:431:THR:CG2	2.50	0.40
1:A:515:ARG:CG	4:A:2009:HOH:O	2.69	0.40
1:A:329:ALA:CA	4:A:2109:HOH:O	2.62	0.40
2:B:441:LEU:HA	2:B:441:LEU:HD12	1.76	0.40
1:A:242:SER:CB	4:A:2014:HOH:O	2.69	0.40
2:B:371:ALA:HB1	2:B:381:PHE:HB2	2.03	0.40
1:A:381:PHE:HZ	2:B:374:ALA:HB2	1.86	0.40
1:A:319:ILE:O	1:A:323:ARG:N	2.52	0.40
1:A:306:GLN:CG	4:A:2074:HOH:O	2.40	0.40
1:A:464:GLU:HA	4:A:2273:HOH:O	2.22	0.40
1:A:366:ASN:CG	4:A:2185:HOH:O	2.59	0.40
1:A:441:LEU:HD13	1:A:441:LEU:HA	1.91	0.40
1:A:412:ILE:HG21	2:B:338:SER:HB2	2.04	0.40
1:A:291:ALA:HA	1:A:462:ILE:HD13	2.02	0.40
1:A:423:ILE:O	1:A:427:VAL:HG23	2.21	0.40
2:B:247:GLU:CB	4:B:2019:HOH:O	2.69	0.40
2:B:288:LYS:HB3	2:B:288:LYS:HE2	1.94	0.40
2:B:404:ARG:CB	4:B:2188:HOH:O	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2166:HOH:O	4:B:2050:HOH:O[1_556]	1.79	0.41

### 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	307/309 (99%)	298 (97%)	8 (3%)	1 (0%)	46	68
2	B	306/309 (99%)	292 (95%)	13 (4%)	1 (0%)	46	68
All	All	613/618 (99%)	590 (96%)	21 (3%)	2 (0%)	46	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	374	ALA
1	A	376	GLU

#### 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	251/253 (99%)	212 (84%)	39 (16%)	3	6
2	B	247/253 (98%)	207 (84%)	40 (16%)	3	5
All	All	498/506 (98%)	419 (84%)	79 (16%)	3	5

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ASP
1	A	228	GLN
1	A	232	PHE
1	A	234	VAL
1	A	251	GLN
1	A	256	SER
1	A	257	LYS
1	A	259	MET
1	A	266	ILE
1	A	270	SER
1	A	302	ASP
1	A	306	GLN
1	A	310	GLU
1	A	313	ASP
1	A	319	ILE
1	A	323	ARG
1	A	347	THR
1	A	348	SER
1	A	354	ASN
1	A	362	LEU
1	A	365	LEU
1	A	366	ASN
1	A	373	ARG
1	A	376	GLU
1	A	411	SER
1	A	414	GLU
1	A	421	SER
1	A	438	ASP
1	A	441	LEU
1	A	454	MET
1	A	455	LEU
1	A	464	GLU
1	A	476	MET
1	A	496	ARG
1	A	504	THR
1	A	505	GLU
1	A	506	GLU
1	A	509	SER
1	A	518	VAL
2	B	226	ASP
2	B	230	GLU
2	B	238	ILE
2	B	240	GLU

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Mol	Chain	Res	Type
2	B	250	ASN
2	B	259	MET
2	B	295	GLN
2	B	306	GLN
2	B	309	LYS
2	B	320	GLU
2	B	321	VAL
2	B	323	ARG
2	B	325	ILE
2	B	330	LYS
2	B	333	GLU
2	B	334	ARG
2	B	347	THR
2	B	351	GLU
2	B	356	ILE
2	B	369	ILE
2	B	376	GLU
2	B	396	GLN
2	B	414	GLU
2	B	415	ASP
2	B	421	SER
2	B	423	ILE
2	B	424	THR
2	B	428	GLU
2	B	438	ASP
2	B	441	LEU
2	B	442	ASN
2	B	444	ILE
2	B	453	GLU
2	B	456	GLN
2	B	462	ILE
2	B	476	MET
2	B	478	GLU
2	B	500	ILE
2	B	517	ASN
2	B	521	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	261	ASN
1	A	303	GLN
1	A	340	GLN
1	A	396	GLN
1	A	465	GLN
1	A	488	ASN
2	B	261	ASN
2	B	397	GLN
2	B	401	ASN
2	B	407	ASN
2	B	452	ASN
2	B	466	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	309/309 (100%)	0.35	21 (6%)	20 23	22, 56, 108, 123	0
2	B	308/309 (99%)	0.38	19 (6%)	24 27	17, 61, 104, 126	0
All	All	617/618 (99%)	0.36	40 (6%)	22 25	17, 59, 107, 126	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	419	VAL	8.1
2	B	528	TYR	5.6
2	B	311	ALA	5.6
1	A	328	SER	5.3
1	A	528	TYR	4.7
1	A	223	HIS	4.6
2	B	224	MET	4.5
1	A	221	GLY	4.3
1	A	375	GLY	4.2
1	A	339	PHE	4.1
2	B	331	ASP	3.9
1	A	522	LYS	3.8
2	B	377	ALA	3.5
1	A	404	ARG	3.4
1	A	330	LYS	3.4
1	A	222	SER	3.4
1	A	224	MET	3.1
1	A	423	ILE	3.1
2	B	349	PHE	3.1
1	A	427	VAL	3.0
1	A	526	ALA	2.8
1	A	323	ARG	2.8
1	A	523	GLU	2.7
1	A	376	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	418	LYS	2.6
1	A	374	ALA	2.6
1	A	324	MET	2.5
2	B	316	LYS	2.5
2	B	329	ALA	2.4
2	B	527	ARG	2.4
1	A	349	PHE	2.4
2	B	374	ALA	2.4
2	B	399	SER	2.3
2	B	381	PHE	2.3
2	B	382	ALA	2.3
2	B	380	GLY	2.2
2	B	529	LYS	2.1
2	B	403	ARG	2.1
2	B	521	LEU	2.1
1	A	400	GLU	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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PB	A	1531	1/1	0.81	0.11	-1.59	100,100,100,100	1
3	PB	A	1530	1/1	0.98	0.10	-	66,66,66,66	1

## 6.5 Other polymers

There are no such residues in this entry.