



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EWD
Title : FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM RABBIT MUSCLE
Authors : Maurady, A.; Sygusch, J.
Deposited on : 2000-04-25
Resolution : 2.46 Å(reported)

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

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

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

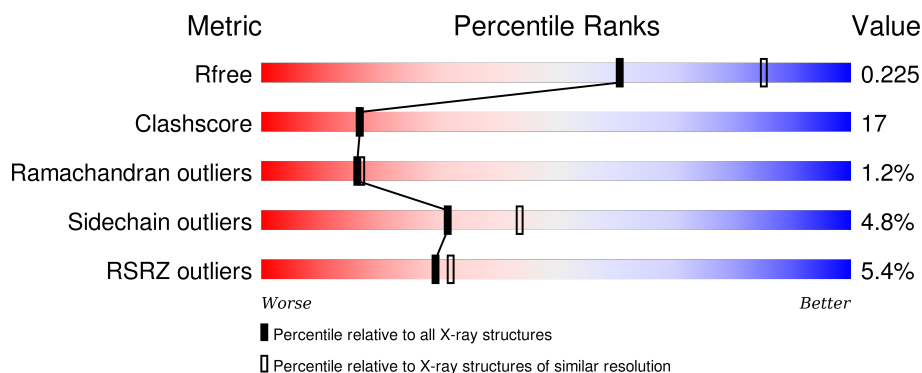
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>5%</div> <div>71%</div> <div>26%</div> <div>••</div> </div>
1	B	363	<div> <div>6%</div> <div>69%</div> <div>29%</div> <div>•</div> </div>
1	C	363	<div> <div>5%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
1	D	363	<div> <div>6%</div> <div>70%</div> <div>27%</div> <div>•</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13358 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 FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2756	1730	488	526	12			
1	B	363	Total	C	N	O	S	0	0	0
			2756	1730	488	526	12			
1	C	363	Total	C	N	O	S	0	0	0
			2756	1730	488	526	12			
1	D	363	Total	C	N	O	S	0	0	0
			2756	1730	488	526	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	LYS	ENGINEERED	UNP P00883
A	344	SER	PRO	CONFLICT	UNP P00883
B	107	MET	LYS	ENGINEERED	UNP P00883
B	344	SER	PRO	CONFLICT	UNP P00883
C	107	MET	LYS	ENGINEERED	UNP P00883
C	344	SER	PRO	CONFLICT	UNP P00883
D	107	MET	LYS	ENGINEERED	UNP P00883
D	344	SER	PRO	CONFLICT	UNP P00883

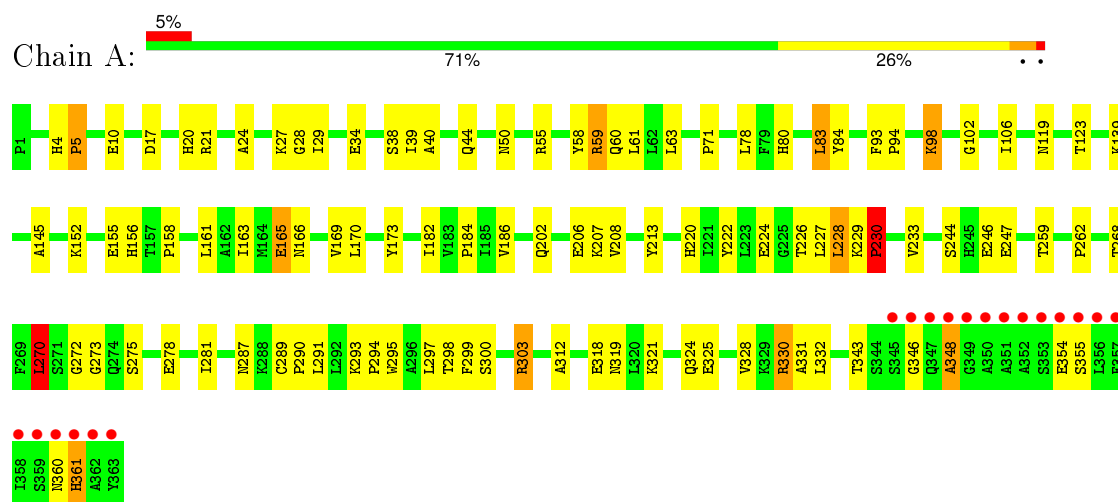
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	544	Total	O	0	0
			544	544		
2	B	494	Total	O	0	0
			494	494		
2	C	676	Total	O	0	0
			676	676		
2	D	620	Total	O	0	0
			620	620		

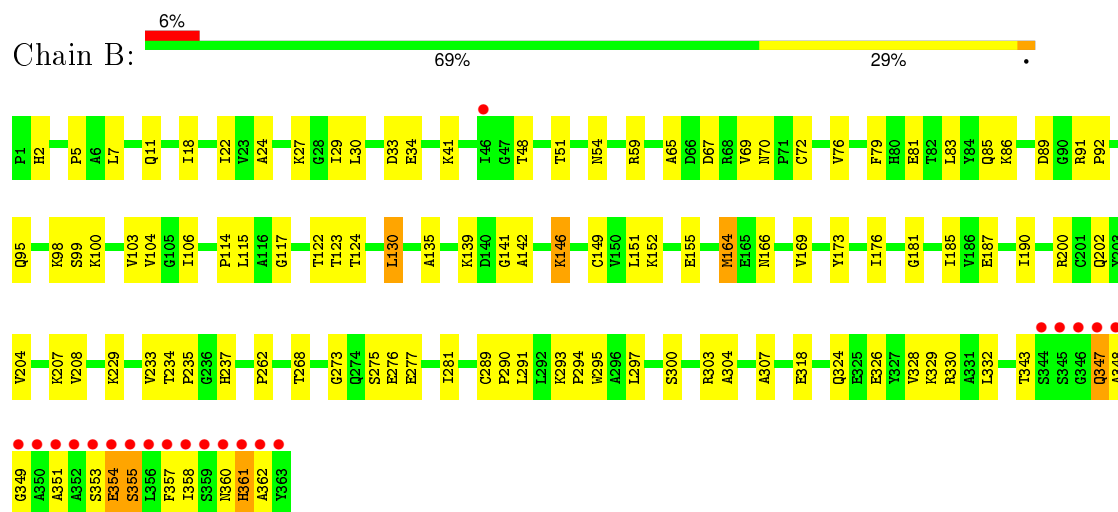
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

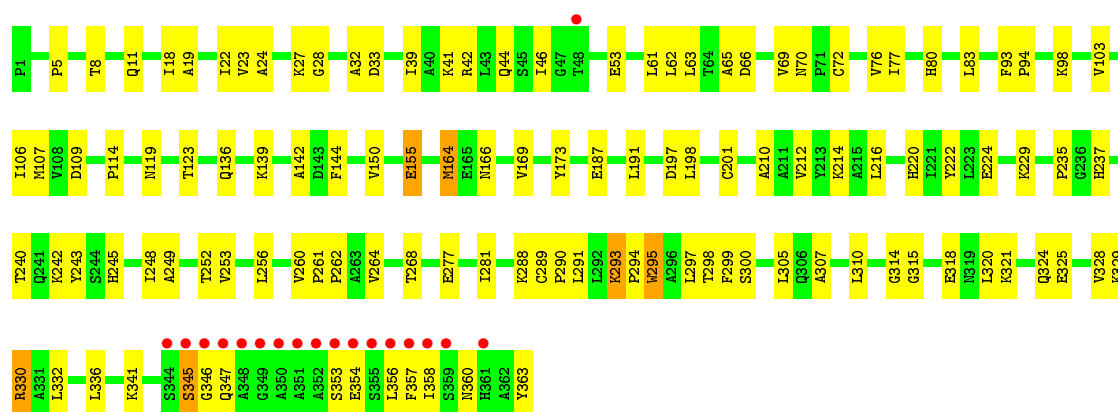


• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

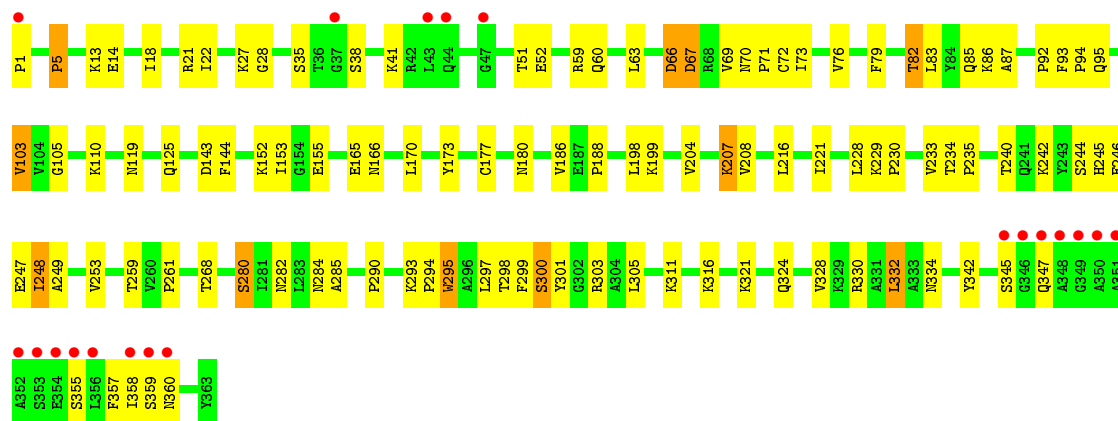


• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE





● Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.19Å 57.58Å 85.35Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	10.00 – 2.46 33.35 – 2.46	Depositor EDS
% Data completeness (in resolution range)	8.0 (10.00-2.46) 68.5 (33.35-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.170 , 0.234 0.165 , 0.225	Depositor DCC
R_{free} test set	3094 reflections (8.13%)	DCC
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	1.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 122.2	EDS
Estimated twinning fraction	0.012 for -h-l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 38915 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13358	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.32	0/2809	0.61	1/3805 (0.0%)
1	B	0.32	0/2809	0.59	0/3805
1	C	0.33	0/2809	0.58	0/3805
1	D	0.31	0/2809	0.59	1/3805 (0.0%)
All	All	0.32	0/11236	0.59	2/15220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LEU	CA-CB-CG	8.12	133.99	115.30
1	D	300	SER	N-CA-C	-5.23	96.89	111.00

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	2756	0	2770	90	0
1	B	2756	0	2770	87	0
1	C	2756	0	2770	113	0
1	D	2756	0	2770	85	0
2	A	544	0	0	35	0
2	B	494	0	0	26	0
2	C	676	0	0	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	620	0	0	40	0
All	All	13358	0	11080	365	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 17.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:HIS:HA	2:C:3465:HOH:O	1.76	0.84
1:A:94:PRO:HD3	2:A:1852:HOH:O	1.80	0.81
1:A:24:ALA:HB3	1:A:27:LYS:HD3	1.63	0.80
1:C:24:ALA:HB3	1:C:27:LYS:HD2	1.63	0.80
1:C:307:ALA:HA	2:C:3937:HOH:O	1.81	0.80
1:D:85:GLN:HA	2:D:5401:HOH:O	1.81	0.79
1:C:155:GLU:HA	2:C:3785:HOH:O	1.81	0.78
1:A:60:GLN:HA	2:A:1802:HOH:O	1.83	0.78
1:C:198:LEU:HA	2:C:3988:HOH:O	1.84	0.78
1:D:166:ASN:HB2	2:D:5920:HOH:O	1.84	0.77
1:A:294:PRO:HD2	2:A:1477:HOH:O	1.84	0.77
1:C:70:ASN:HB3	2:C:3380:HOH:O	1.85	0.77
1:D:177:CYS:HA	2:D:5807:HOH:O	1.85	0.76
1:B:22:ILE:HG12	1:B:103:VAL:HG21	1.67	0.76
1:C:353:SER:HB3	2:C:3374:HOH:O	1.87	0.74
1:C:44:GLN:HB3	2:C:3849:HOH:O	1.86	0.73
1:B:328:VAL:HA	2:B:2728:HOH:O	1.88	0.73
1:B:276:GLU:HB2	1:B:351:ALA:HB1	1.70	0.73
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.70	0.73
1:C:80:HIS:HB3	2:C:4018:HOH:O	1.88	0.72
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.71	0.72
1:A:184:PRO:HG2	1:A:226:THR:HG22	1.72	0.72
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.71	0.71
1:C:242:LYS:HE2	1:C:358:ILE:HG21	1.72	0.70
1:A:318:GLU:HB2	2:A:1671:HOH:O	1.89	0.70
1:B:79:PHE:HD1	1:B:81:GLU:HG2	1.56	0.70
1:D:204:VAL:HB	2:D:5939:HOH:O	1.91	0.70
1:C:330:ARG:HA	1:C:330:ARG:HE	1.55	0.70
1:D:321:LYS:HG3	2:D:5784:HOH:O	1.91	0.70
1:C:61:LEU:HA	2:C:3676:HOH:O	1.91	0.70
1:D:204:VAL:O	1:D:208:VAL:HG23	1.91	0.69
1:B:273:GLY:HA2	1:B:303:ARG:HH12	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HG3	2:A:1693:HOH:O	1.94	0.68
1:D:290:PRO:HD3	2:D:5795:HOH:O	1.94	0.68
1:B:106:ILE:HB	2:B:2769:HOH:O	1.94	0.68
1:D:285:ALA:HB3	2:D:5573:HOH:O	1.94	0.67
1:C:248:ILE:HD11	2:C:3869:HOH:O	1.93	0.67
1:D:242:LYS:HB3	2:D:5365:HOH:O	1.95	0.67
1:A:328:VAL:O	1:A:332:LEU:HG	1.95	0.67
1:C:139:LYS:HD3	2:C:3404:HOH:O	1.95	0.66
1:C:240:THR:HG22	1:C:357:PHE:O	1.96	0.66
1:B:135:ALA:HA	2:B:2643:HOH:O	1.97	0.65
1:C:46:ILE:HB	1:C:314:GLY:HA2	1.78	0.65
1:B:303:ARG:HD3	2:B:2694:HOH:O	1.97	0.65
1:C:155:GLU:HB2	2:C:3911:HOH:O	1.97	0.65
1:C:321:LYS:HD2	2:C:3976:HOH:O	1.97	0.65
1:C:72:CYS:SG	1:C:332:LEU:HD23	2.38	0.63
1:C:150:VAL:HG13	1:C:191:LEU:HD13	1.80	0.63
1:C:294:PRO:HB3	2:C:3736:HOH:O	1.99	0.63
1:B:142:ALA:HB2	2:B:2645:HOH:O	1.99	0.63
1:B:155:GLU:HA	2:C:2709:HOH:O	1.99	0.62
1:C:330:ARG:NE	1:C:330:ARG:HA	2.13	0.62
1:A:83:LEU:HD21	2:A:1485:HOH:O	1.98	0.62
1:A:186:VAL:HG22	2:A:1624:HOH:O	1.99	0.62
1:B:41:LYS:HB2	2:B:2768:HOH:O	1.98	0.62
1:D:207:LYS:HD2	1:D:207:LYS:N	2.15	0.62
1:B:294:PRO:HG2	1:C:262:PRO:CG	2.30	0.62
1:C:347:GLN:HG2	2:C:3782:HOH:O	1.99	0.62
1:B:357:PHE:HB2	1:B:360:ASN:OD1	2.00	0.62
1:B:268:THR:HB	1:B:300:SER:HB2	1.82	0.61
1:B:326:GLU:HA	1:B:329:LYS:HD3	1.83	0.61
1:C:103:VAL:HG23	1:C:144:PHE:CE2	2.36	0.61
1:A:94:PRO:HB2	2:A:1661:HOH:O	2.00	0.60
1:B:293:LYS:HG2	1:B:297:LEU:CD1	2.30	0.60
1:A:270:LEU:HD22	1:A:272:GLY:H	1.65	0.60
1:B:34:GLU:HB2	1:B:59:ARG:NH2	2.17	0.60
1:D:152:LYS:HD2	2:D:5711:HOH:O	2.01	0.59
1:D:268:THR:HB	1:D:300:SER:HB2	1.84	0.59
1:A:268:THR:HB	1:A:300:SER:HB2	1.83	0.59
1:A:93:PHE:HB2	2:A:1852:HOH:O	2.02	0.59
1:A:161:LEU:O	1:A:165:GLU:HB2	2.02	0.59
1:B:349:GLY:HA3	2:B:2734:HOH:O	2.01	0.59
1:C:22:ILE:HG12	1:C:103:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HG2	1:A:297:LEU:CD1	2.33	0.58
1:A:321:LYS:HB2	2:A:1542:HOH:O	2.03	0.58
1:A:4:HIS:O	1:B:117:GLY:HA2	2.04	0.58
1:A:17:ASP:HB3	2:A:1662:HOH:O	2.03	0.58
1:C:63:LEU:HD21	1:C:76:VAL:HG11	1.85	0.57
1:D:180:ASN:HB2	2:D:5807:HOH:O	2.03	0.57
1:B:273:GLY:HA2	1:B:303:ARG:NH1	2.19	0.57
1:B:99:SER:HB2	2:B:2750:HOH:O	2.04	0.57
1:A:27:LYS:HG2	1:A:71:PRO:O	2.04	0.57
1:B:22:ILE:HG12	1:B:103:VAL:CG2	2.34	0.57
1:D:240:THR:HG22	1:D:357:PHE:O	2.03	0.57
1:C:249:ALA:O	1:C:253:VAL:HG23	2.04	0.57
1:C:293:LYS:HG2	1:C:297:LEU:HD11	1.85	0.56
1:A:123:THR:HA	1:A:166:ASN:OD1	2.05	0.56
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.86	0.56
1:D:83:LEU:HA	2:D:5765:HOH:O	2.05	0.56
1:A:59:ARG:O	1:A:63:LEU:HG	2.05	0.56
1:C:318:GLU:HB3	2:C:3932:HOH:O	2.05	0.56
1:D:76:VAL:HG13	2:D:5918:HOH:O	2.05	0.56
1:A:324:GLN:O	1:A:328:VAL:HG23	2.05	0.56
1:D:86:LYS:HE3	2:D:5983:HOH:O	2.06	0.56
1:D:110:LYS:HB2	1:D:125:GLN:HG3	1.87	0.56
1:A:355:SER:HA	2:A:1842:HOH:O	2.05	0.56
1:C:341:LYS:HB3	2:C:3383:HOH:O	2.05	0.56
1:C:356:LEU:HD12	2:C:3893:HOH:O	2.06	0.56
1:D:295:TRP:HZ3	2:D:5732:HOH:O	1.88	0.55
1:A:155:GLU:HG3	2:C:1640:HOH:O	2.06	0.55
1:D:94:PRO:HD3	2:D:5765:HOH:O	2.05	0.55
1:A:348:ALA:HB3	2:A:1896:HOH:O	2.06	0.55
1:B:114:PRO:HA	1:B:122:THR:HG22	1.89	0.55
1:D:303:ARG:HG2	2:D:5863:HOH:O	2.07	0.55
1:B:83:LEU:HD21	2:B:2645:HOH:O	2.07	0.55
1:A:360:ASN:HA	2:A:1740:HOH:O	2.07	0.54
1:C:32:ALA:HB2	2:C:3733:HOH:O	2.05	0.54
1:C:41:LYS:H	1:C:41:LYS:HD2	1.72	0.54
1:A:228:LEU:O	1:A:230:PRO:HD3	2.07	0.54
1:B:358:ILE:HG13	1:B:358:ILE:O	2.08	0.54
1:A:158:PRO:O	1:D:1:PRO:HD3	2.07	0.54
1:B:277:GLU:HG3	1:B:281:ILE:HD11	1.88	0.54
1:C:142:ALA:HB2	2:C:3975:HOH:O	2.07	0.54
1:C:39:ILE:HD12	1:C:42:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:VAL:HG11	1:C:293:LYS:HD2	1.90	0.53
1:D:234:THR:HG22	1:D:248:ILE:HG13	1.90	0.53
1:C:201:CYS:HB3	2:C:3988:HOH:O	2.08	0.53
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.06	0.53
1:A:155:GLU:HG2	1:A:156:HIS:CE1	2.43	0.53
1:C:291:LEU:O	1:C:293:LYS:HD3	2.09	0.53
1:A:325:GLU:HB3	2:A:1642:HOH:O	2.07	0.53
1:A:291:LEU:O	1:A:293:LYS:HD3	2.09	0.53
1:D:170:LEU:HD22	1:D:186:VAL:HG13	1.91	0.53
1:A:246:GLU:HB2	2:A:1580:HOH:O	2.09	0.53
1:D:311:LYS:HE3	2:D:5942:HOH:O	2.08	0.53
1:C:222:TYR:CZ	1:C:224:GLU:HB2	2.44	0.53
1:B:276:GLU:HB2	1:B:351:ALA:CB	2.38	0.52
1:A:80:HIS:HA	2:A:1440:HOH:O	2.07	0.52
1:B:360:ASN:HB3	2:B:2632:HOH:O	2.08	0.52
1:C:320:LEU:HD23	2:C:3967:HOH:O	2.08	0.52
1:D:355:SER:HA	2:D:5828:HOH:O	2.08	0.52
1:B:79:PHE:CD1	1:B:81:GLU:HG2	2.41	0.52
1:B:362:ALA:HA	2:B:2743:HOH:O	2.09	0.51
1:A:78:LEU:O	1:A:106:ILE:HD12	2.10	0.51
1:A:83:LEU:HD22	2:A:1440:HOH:O	2.10	0.51
1:D:35:SER:HA	1:D:79:PHE:CE2	2.46	0.51
1:A:63:LEU:HB2	2:A:1802:HOH:O	2.10	0.51
1:C:293:LYS:HG2	1:C:297:LEU:CD1	2.41	0.50
1:C:354:GLU:HG2	2:C:4015:HOH:O	2.11	0.50
1:A:346:GLY:HA2	2:A:1825:HOH:O	2.11	0.50
1:C:336:LEU:HD22	1:C:341:LYS:HG3	1.93	0.50
1:C:252:THR:O	1:C:256:LEU:HD23	2.11	0.50
1:D:332:LEU:HD13	2:D:5525:HOH:O	2.11	0.50
1:D:359:SER:HB2	2:D:5915:HOH:O	2.11	0.50
1:A:303:ARG:NH2	1:A:354:GLU:HG3	2.26	0.50
1:D:301:TYR:CB	1:D:305:LEU:HG	2.41	0.50
1:D:95:GLN:HG3	2:D:5712:HOH:O	2.12	0.50
1:B:190:ILE:HD13	1:B:204:VAL:HG12	1.94	0.50
1:C:268:THR:HG22	1:C:298:THR:HG23	1.94	0.50
1:B:291:LEU:O	1:B:293:LYS:HD3	2.12	0.50
1:C:289:CYS:SG	1:C:291:LEU:HD23	2.52	0.50
1:D:27:LYS:HA	1:D:72:CYS:O	2.12	0.50
1:B:361:HIS:O	1:B:361:HIS:CG	2.65	0.50
1:B:330:ARG:NE	1:B:330:ARG:HA	2.27	0.50
1:B:294:PRO:HG2	1:C:262:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ASN:ND2	1:D:342:TYR:H	2.09	0.50
1:A:83:LEU:HD23	1:A:84:TYR:CE2	2.47	0.49
1:C:83:LEU:HD11	2:C:3975:HOH:O	2.12	0.49
1:D:38:SER:HA	1:D:41:LYS:HE3	1.94	0.49
1:A:21:ARG:HD3	2:A:1662:HOH:O	2.12	0.49
1:D:244:SER:OG	1:D:247:GLU:HG3	2.12	0.49
1:D:52:GLU:HG2	2:D:5393:HOH:O	2.12	0.49
1:C:27:LYS:HE3	2:C:3924:HOH:O	2.12	0.49
1:D:360:ASN:HB3	2:D:5642:HOH:O	2.12	0.49
1:A:208:VAL:HG13	2:A:1660:HOH:O	2.12	0.49
1:D:67:ASP:HA	1:D:70:ASN:OD1	2.13	0.49
1:C:164:MET:HA	2:C:4024:HOH:O	2.12	0.49
1:B:139:LYS:HG3	2:B:2718:HOH:O	2.12	0.49
1:B:104:VAL:HB	1:B:141:GLY:O	2.12	0.49
1:A:343:THR:HB	2:A:5909:HOH:O	2.12	0.49
1:C:22:ILE:HG12	1:C:103:VAL:CG2	2.44	0.48
1:C:281:ILE:HD12	2:C:3830:HOH:O	2.12	0.48
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.42	0.48
1:C:245:HIS:CE1	1:C:346:GLY:HA3	2.49	0.48
1:B:149:CYS:HB3	2:B:2812:HOH:O	2.14	0.48
1:C:310:LEU:HD23	2:C:3937:HOH:O	2.12	0.48
1:D:13:LYS:HG2	2:D:5825:HOH:O	2.12	0.48
1:C:363:TYR:HA	2:C:3467:HOH:O	2.12	0.48
1:A:330:ARG:NH1	1:A:330:ARG:HG3	2.27	0.48
1:C:341:LYS:HE2	2:C:2431:HOH:O	2.14	0.48
1:A:244:SER:OG	1:A:247:GLU:HG3	2.14	0.48
1:C:320:LEU:HD11	2:C:3676:HOH:O	2.14	0.48
1:B:181:GLY:HA2	2:B:2380:HOH:O	2.13	0.48
1:D:233:VAL:O	1:D:248:ILE:HG12	2.14	0.47
1:B:7:LEU:HA	1:B:11:GLN:OE1	2.14	0.47
1:D:103:VAL:HG23	1:D:143:ASP:HB2	1.95	0.47
1:B:5:PRO:HD3	2:B:2817:HOH:O	2.12	0.47
1:B:237:HIS:HD2	2:B:2670:HOH:O	1.96	0.47
1:B:81:GLU:O	1:B:85:GLN:HG3	2.14	0.47
1:A:287:ASN:HB3	2:A:5504:HOH:O	2.13	0.47
1:A:39:ILE:HG21	1:A:55:ARG:CD	2.43	0.47
1:B:275:SER:HB2	1:B:351:ALA:O	2.14	0.47
1:D:153:ILE:HD11	2:D:5939:HOH:O	2.14	0.47
1:A:330:ARG:HH11	1:A:330:ARG:HG3	1.80	0.47
1:B:324:GLN:O	1:B:328:VAL:HG23	2.15	0.47
1:D:93:PHE:N	1:D:94:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:O	1:A:259:THR:HG21	2.14	0.47
1:B:92:PRO:HG2	1:B:95:GLN:HG3	1.95	0.47
1:C:166:ASN:O	1:C:169:VAL:HG12	2.15	0.47
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.50	0.47
1:D:321:LYS:HE2	2:D:5860:HOH:O	2.15	0.46
1:C:61:LEU:HD23	1:C:324:GLN:HG2	1.96	0.46
1:B:329:LYS:HG2	2:B:3446:HOH:O	2.15	0.46
1:A:348:ALA:HB2	2:A:1448:HOH:O	2.14	0.46
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.97	0.46
1:A:202:GLN:HB2	1:A:233:VAL:HG11	1.95	0.46
1:C:41:LYS:HE3	2:C:3825:HOH:O	2.15	0.46
1:A:58:TYR:O	1:A:61:LEU:HB3	2.15	0.46
1:B:83:LEU:HG	2:B:2611:HOH:O	2.15	0.46
1:C:62:LEU:HD13	2:C:3733:HOH:O	2.15	0.46
1:D:358:ILE:HD12	1:D:358:ILE:N	2.31	0.46
1:C:315:GLY:HA3	2:C:4029:HOH:O	2.14	0.46
1:D:282:ASN:HA	2:D:5573:HOH:O	2.15	0.46
1:D:51:THR:HG22	2:D:5393:HOH:O	2.15	0.46
1:B:207:LYS:NZ	1:C:220:HIS:HD2	2.14	0.46
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.98	0.46
1:D:69:VAL:HG13	1:D:328:VAL:HG22	1.97	0.46
1:C:66:ASP:O	1:C:69:VAL:HG22	2.16	0.46
1:C:93:PHE:N	1:C:94:PRO:HD2	2.31	0.46
1:A:24:ALA:HB3	1:A:27:LYS:CD	2.41	0.46
1:C:245:HIS:HE1	1:C:346:GLY:HA3	1.81	0.46
1:D:82:THR:HG22	1:D:93:PHE:HD2	1.80	0.46
1:A:213:TYR:OH	1:A:228:LEU:HG	2.16	0.46
1:C:289:CYS:O	1:C:293:LYS:HE3	2.15	0.45
1:A:20:HIS:CD2	2:A:1805:HOH:O	2.68	0.45
1:B:115:LEU:HD21	1:B:123:THR:OG1	2.16	0.45
1:D:229:LYS:HG3	1:D:268:THR:O	2.16	0.45
1:B:149:CYS:CB	2:B:2812:HOH:O	2.65	0.45
1:D:72:CYS:SG	1:D:332:LEU:HD12	2.57	0.45
1:C:123:THR:HG23	2:D:4006:HOH:O	2.17	0.45
1:A:94:PRO:O	1:A:98:LYS:HG2	2.15	0.45
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.51	0.45
1:A:331:ALA:HB3	2:A:1551:HOH:O	2.15	0.45
1:C:136:GLN:O	1:C:139:LYS:HB3	2.15	0.45
1:A:229:LYS:HG3	1:A:268:THR:O	2.16	0.45
1:C:253:VAL:HB	2:C:3909:HOH:O	2.17	0.45
1:D:92:PRO:HB2	1:D:94:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:HH11	1:A:330:ARG:HA	1.82	0.45
1:B:72:CYS:SG	1:B:332:LEU:HD23	2.57	0.45
1:D:198:LEU:HB3	1:D:199:LYS:NZ	2.32	0.45
1:A:10:GLU:HB3	2:A:1839:HOH:O	2.17	0.45
1:D:83:LEU:HD12	2:D:5765:HOH:O	2.16	0.45
1:D:66:ASP:O	1:D:69:VAL:HG22	2.17	0.45
1:B:86:LYS:HE3	1:B:92:PRO:HD3	1.98	0.45
1:C:187:GLU:HG3	1:C:229:LYS:O	2.16	0.44
1:B:347:GLN:HG3	2:B:2412:HOH:O	2.17	0.44
1:D:246:GLU:HG3	2:D:5728:HOH:O	2.17	0.44
1:D:249:ALA:O	1:D:253:VAL:HG23	2.17	0.44
1:B:33:ASP:OD2	1:B:146:LYS:HE3	2.16	0.44
1:C:325:GLU:HG3	1:C:329:LYS:HZ2	1.83	0.44
1:C:260:VAL:HG13	1:C:264:VAL:HG21	1.99	0.44
1:C:214:LYS:HE3	2:C:2720:HOH:O	2.17	0.44
1:A:145:ALA:HB2	1:A:182:ILE:HG21	1.99	0.44
1:B:70:ASN:OD1	1:B:100:LYS:HE2	2.17	0.44
1:A:161:LEU:HD21	2:B:2716:HOH:O	2.17	0.44
1:C:291:LEU:H	1:C:291:LEU:HD22	1.83	0.44
1:C:103:VAL:HG23	1:C:144:PHE:HE2	1.80	0.44
1:B:361:HIS:HB3	2:B:2810:HOH:O	2.17	0.44
1:A:170:LEU:HD13	1:A:186:VAL:HG12	1.99	0.44
1:D:198:LEU:HB3	1:D:199:LYS:HZ2	1.81	0.44
1:A:270:LEU:HD22	1:A:272:GLY:N	2.32	0.44
1:A:98:LYS:HA	1:A:102:GLY:O	2.18	0.44
1:A:268:THR:HG22	1:A:298:THR:HG23	1.99	0.44
1:C:65:ALA:HB1	2:C:4010:HOH:O	2.18	0.44
1:C:288:LYS:HE2	2:C:3714:HOH:O	2.16	0.44
1:C:277:GLU:O	1:C:281:ILE:HG13	2.17	0.43
1:A:262:PRO:CG	1:D:294:PRO:HG2	2.47	0.43
1:C:237:HIS:HE1	2:C:3833:HOH:O	2.00	0.43
1:A:361:HIS:CD2	2:A:1704:HOH:O	2.70	0.43
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.53	0.43
1:C:235:PRO:HG2	2:C:3587:HOH:O	2.19	0.43
1:B:29:ILE:HB	1:B:300:SER:HA	2.00	0.43
1:D:280:SER:HB3	1:D:334:ASN:OD1	2.18	0.43
1:C:360:ASN:HB2	2:C:4008:HOH:O	2.17	0.43
1:B:354:GLU:O	1:B:355:SER:HB2	2.18	0.43
1:A:152:LYS:HE3	1:A:152:LYS:HB2	1.68	0.43
1:D:305:LEU:HD22	2:D:5534:HOH:O	2.18	0.43
1:B:277:GLU:HG2	1:B:348:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:THR:OG1	1:C:11:GLN:HG3	2.18	0.43
1:B:289:CYS:O	1:B:293:LYS:NZ	2.51	0.43
1:A:163:ILE:HG23	2:A:1660:HOH:O	2.17	0.43
1:D:297:LEU:HD11	2:D:5732:HOH:O	2.17	0.43
1:A:330:ARG:HH11	1:A:330:ARG:CG	2.32	0.43
1:B:86:LYS:HG2	1:B:92:PRO:HA	2.01	0.43
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.89	0.43
1:A:207:LYS:HG3	2:D:5788:HOH:O	2.18	0.43
1:B:30:LEU:HB3	1:B:76:VAL:HG22	2.01	0.43
1:C:347:GLN:HG3	1:C:347:GLN:O	2.18	0.43
1:A:29:ILE:CD1	1:A:268:THR:HG21	2.48	0.43
1:C:354:GLU:HB2	2:C:3392:HOH:O	2.19	0.43
1:D:216:LEU:HD22	1:D:221:ILE:HG13	2.01	0.43
1:D:268:THR:HG22	1:D:298:THR:HG23	2.01	0.43
1:D:60:GLN:NE2	1:D:87:ALA:HA	2.34	0.43
1:A:281:ILE:HD12	2:A:1809:HOH:O	2.18	0.43
1:C:291:LEU:N	1:C:291:LEU:HD22	2.34	0.42
1:A:39:ILE:HG21	1:A:55:ARG:HD3	2.00	0.42
1:B:166:ASN:O	1:B:169:VAL:HG12	2.19	0.42
1:B:289:CYS:HA	1:B:290:PRO:HD3	1.81	0.42
1:D:316:LYS:HB3	2:D:5811:HOH:O	2.18	0.42
1:D:14:GLU:O	1:D:18:ILE:HG13	2.19	0.42
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.54	0.42
1:A:222:TYR:CZ	1:A:224:GLU:HB2	2.54	0.42
1:D:324:GLN:HB3	2:D:5917:HOH:O	2.19	0.42
1:D:245:HIS:HA	2:D:5390:HOH:O	2.19	0.42
1:C:114:PRO:HB3	2:C:3863:HOH:O	2.18	0.42
1:D:59:ARG:O	1:D:63:LEU:HG	2.20	0.42
1:B:262:PRO:HG3	1:C:262:PRO:HG3	2.02	0.42
1:C:235:PRO:HA	2:C:3988:HOH:O	2.19	0.42
1:B:262:PRO:HG3	1:C:294:PRO:HG3	2.02	0.42
1:C:261:PRO:HA	1:C:262:PRO:HD3	1.95	0.42
1:A:321:LYS:HD2	2:A:1663:HOH:O	2.18	0.42
1:C:229:LYS:HE2	1:C:300:SER:HB3	2.00	0.42
1:D:103:VAL:HG22	1:D:144:PHE:CD2	2.54	0.42
1:A:275:SER:OG	1:A:278:GLU:HB2	2.19	0.42
1:C:305:LEU:HD23	1:C:330:ARG:HB3	2.02	0.42
1:C:103:VAL:HG23	1:C:144:PHE:CD2	2.54	0.42
1:D:105:GLY:HA2	1:D:144:PHE:O	2.19	0.42
1:B:123:THR:HG22	1:B:124:THR:N	2.35	0.42
1:C:291:LEU:HB2	2:C:3909:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:HB3	2:B:2650:HOH:O	2.20	0.42
1:D:18:ILE:O	1:D:22:ILE:HG13	2.20	0.42
1:A:273:GLY:CA	2:A:1869:HOH:O	2.67	0.42
1:A:139:LYS:O	1:A:139:LYS:HD2	2.20	0.42
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.20	0.41
1:A:29:ILE:HD12	1:A:268:THR:HG21	2.01	0.41
1:A:208:VAL:HG22	2:A:1660:HOH:O	2.19	0.41
1:B:51:THR:HG23	1:B:54:ASN:HB2	2.02	0.41
1:C:328:VAL:HG23	2:C:4010:HOH:O	2.20	0.41
1:A:38:SER:HB3	2:A:1652:HOH:O	2.19	0.41
1:B:130:LEU:HB3	1:B:176:ILE:HG21	2.01	0.41
1:D:235:PRO:HD3	2:D:5471:HOH:O	2.19	0.41
1:A:40:ALA:HB2	1:A:50:ASN:ND2	2.35	0.41
1:B:234:THR:HB	1:B:235:PRO:HD2	2.01	0.41
1:C:235:PRO:HG3	1:C:243:TYR:CD1	2.55	0.41
1:D:332:LEU:HD12	1:D:332:LEU:HA	1.90	0.41
1:C:294:PRO:HG2	1:C:295:TRP:CE2	2.56	0.41
1:B:24:ALA:HB3	1:B:27:LYS:HD2	2.01	0.41
1:B:281:ILE:HD13	2:B:2646:HOH:O	2.19	0.41
1:C:210:ALA:HA	2:C:3411:HOH:O	2.20	0.41
1:B:146:LYS:HD3	1:B:187:GLU:OE2	2.20	0.41
1:C:325:GLU:HG3	1:C:329:LYS:NZ	2.35	0.41
1:A:312:ALA:O	1:A:319:ASN:HB3	2.19	0.41
1:C:212:VAL:O	1:C:216:LEU:HG	2.21	0.41
1:C:18:ILE:O	1:C:22:ILE:HG13	2.20	0.41
1:C:83:LEU:HA	1:C:83:LEU:HD12	1.88	0.41
1:B:65:ALA:HB3	1:B:69:VAL:HG11	2.03	0.41
1:A:34:GLU:HB2	1:A:59:ARG:NH1	2.36	0.41
1:B:190:ILE:HD11	1:B:208:VAL:HG21	2.03	0.41
1:B:89:ASP:OD2	1:B:91:ARG:HB2	2.21	0.41
1:B:202:GLN:HB2	1:B:233:VAL:HG11	2.02	0.41
1:C:98:LYS:HD3	2:C:3796:HOH:O	2.21	0.41
1:C:289:CYS:HA	1:C:290:PRO:HD3	1.86	0.41
1:B:151:LEU:HD11	2:B:2650:HOH:O	2.20	0.41
1:B:18:ILE:O	1:B:22:ILE:HG13	2.20	0.40
1:D:293:LYS:HG2	1:D:297:LEU:HD11	2.02	0.40
1:D:92:PRO:C	1:D:94:PRO:HD2	2.42	0.40
1:C:345:SER:HA	2:C:3957:HOH:O	2.22	0.40
1:C:268:THR:HB	1:C:300:SER:HB2	2.03	0.40
1:C:19:ALA:O	1:C:23:VAL:HG22	2.21	0.40
1:B:27:LYS:HA	1:B:72:CYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:MET:HE2	2:D:2751:HOH:O	2.21	0.40
1:D:259:THR:O	1:D:261:PRO:HD3	2.20	0.40
1:D:360:ASN:HB2	2:D:5684:HOH:O	2.21	0.40
1:B:185:ILE:CG2	1:B:229:LYS:HB2	2.51	0.40
1:B:152:LYS:HD3	2:B:2494:HOH: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	361/363 (99%)	331 (92%)	26 (7%)	4 (1%)	17	19
1	B	361/363 (99%)	332 (92%)	23 (6%)	6 (2%)	11	10
1	C	361/363 (99%)	325 (90%)	34 (9%)	2 (1%)	30	35
1	D	361/363 (99%)	337 (93%)	19 (5%)	5 (1%)	14	13
All	All	1444/1452 (99%)	1325 (92%)	102 (7%)	17 (1%)	16	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS
1	B	353	SER
1	B	354	GLU
1	C	345	SER
1	D	5	PRO
1	D	66	ASP
1	D	67	ASP
1	A	348	ALA
1	D	345	SER
1	A	5	PRO

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Mol	Chain	Res	Type
1	B	307	ALA
1	B	355	SER
1	B	67	ASP
1	B	304	ALA
1	A	230	PRO
1	C	5	PRO
1	D	188	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/291 (100%)	275 (94%)	16 (6%)	27	37
1	B	291/291 (100%)	278 (96%)	13 (4%)	34	47
1	C	291/291 (100%)	280 (96%)	11 (4%)	40	55
1	D	291/291 (100%)	275 (94%)	16 (6%)	27	37
All	All	1164/1164 (100%)	1108 (95%)	56 (5%)	31	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	44	GLN
1	A	59	ARG
1	A	83	LEU
1	A	98	LYS
1	A	119	ASN
1	A	165	GLU
1	A	169	VAL
1	A	173	TYR
1	A	227	LEU
1	A	228	LEU
1	A	230	PRO
1	A	270	LEU
1	A	295	TRP

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Mol	Chain	Res	Type
1	A	303	ARG
1	A	330	ARG
1	B	2	HIS
1	B	48	THR
1	B	98	LYS
1	B	130	LEU
1	B	146	LYS
1	B	164	MET
1	B	173	TYR
1	B	200	ARG
1	B	295	TRP
1	B	318	GLU
1	B	343	THR
1	B	347	GLN
1	B	361	HIS
1	C	53	GLU
1	C	106	ILE
1	C	107	MET
1	C	109	ASP
1	C	119	ASN
1	C	155	GLU
1	C	164	MET
1	C	173	TYR
1	C	293	LYS
1	C	295	TRP
1	C	330	ARG
1	D	5	PRO
1	D	21	ARG
1	D	73	ILE
1	D	82	THR
1	D	103	VAL
1	D	119	ASN
1	D	155	GLU
1	D	165	GLU
1	D	173	TYR
1	D	207	LYS
1	D	248	ILE
1	D	280	SER
1	D	295	TRP
1	D	330	ARG
1	D	332	LEU
1	D	347	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	119	ASN
1	A	220	HIS
1	A	241	GLN
1	A	245	HIS
1	B	85	GLN
1	B	136	GLN
1	B	219	HIS
1	B	220	HIS
1	B	237	HIS
1	B	339	GLN
1	C	44	GLN
1	C	119	ASN
1	C	136	GLN
1	C	166	ASN
1	C	220	HIS
1	C	237	HIS
1	C	241	GLN
1	C	245	HIS
1	D	4	HIS
1	D	60	GLN
1	D	85	GLN
1	D	202	GLN
1	D	241	GLN
1	D	284	ASN
1	D	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	363/363 (100%)	-0.18	19 (5%)	31 34	2, 7, 60, 92	0
1	B	363/363 (100%)	-0.24	21 (5%)	26 29	2, 6, 55, 87	0
1	C	363/363 (100%)	-0.25	18 (4%)	32 36	2, 6, 48, 81	0
1	D	363/363 (100%)	-0.31	20 (5%)	29 31	2, 8, 51, 94	0
All	All	1452/1452 (100%)	-0.24	78 (5%)	29 32	2, 7, 55, 94	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	11.1
1	A	359	SER	10.6
1	D	350	ALA	10.1
1	A	355	SER	10.1
1	A	362	ALA	9.2
1	B	350	ALA	8.7
1	B	363	TYR	8.4
1	A	363	TYR	8.2
1	C	345	SER	8.0
1	B	355	SER	7.8
1	B	360	ASN	7.5
1	C	350	ALA	7.3
1	C	351	ALA	7.2
1	A	352	ALA	7.0
1	C	346	GLY	6.9
1	A	357	PHE	6.8
1	B	346	GLY	6.7
1	C	347	GLN	6.7
1	A	353	SER	6.3
1	C	355	SER	6.3
1	C	353	SER	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	6.2
1	A	349	GLY	6.2
1	B	347	GLN	6.2
1	B	362	ALA	6.2
1	B	348	ALA	6.2
1	A	346	GLY	6.0
1	A	360	ASN	6.0
1	D	349	GLY	6.0
1	B	357	PHE	5.9
1	B	356	LEU	5.9
1	B	345	SER	5.7
1	B	359	SER	5.5
1	A	347	GLN	5.5
1	C	349	GLY	5.4
1	A	361	HIS	5.3
1	D	351	ALA	5.2
1	B	361	HIS	5.2
1	D	355	SER	5.2
1	B	351	ALA	5.1
1	C	354	GLU	4.9
1	C	357	PHE	4.8
1	C	344	SER	4.6
1	A	354	GLU	4.5
1	A	358	ILE	4.5
1	A	350	ALA	4.4
1	B	358	ILE	4.4
1	B	349	GLY	4.4
1	B	353	SER	4.3
1	D	346	GLY	4.2
1	B	354	GLU	4.2
1	D	353	SER	4.1
1	C	358	ILE	4.0
1	D	360	ASN	3.9
1	C	359	SER	3.9
1	D	348	ALA	3.8
1	B	352	ALA	3.8
1	D	354	GLU	3.7
1	D	356	LEU	3.7
1	C	356	LEU	3.7
1	A	345	SER	3.5
1	D	358	ILE	3.4
1	A	351	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	348	ALA	3.1
1	D	345	SER	2.8
1	B	344	SER	2.7
1	D	43	LEU	2.6
1	D	352	ALA	2.5
1	D	347	GLN	2.4
1	C	352	ALA	2.4
1	D	359	SER	2.3
1	D	47	GLY	2.3
1	D	1	PRO	2.3
1	C	48	THR	2.2
1	D	44	GLN	2.2
1	D	37	GLY	2.2
1	C	361	HIS	2.1
1	B	46	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.