



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 01:43 PM EDT

PDB ID : 2PHD  
Title : Crystal Structure Determination of a Salicylate 1,2-Dioxygenase from *Pseudomonas salicylatoxidans*  
Authors : Matera, I.; Ferraroni, M.; Briganti, F.  
Deposited on : 2007-04-11  
Resolution : 2.90 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

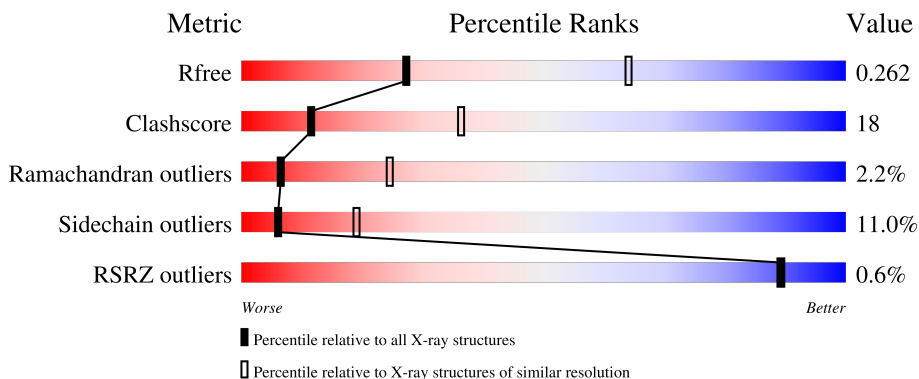
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	368	 66% 24% 5% 5%
1	B	368	 62% 25% 8% 5%
1	C	368	 64% 25% 6% 5%
1	D	368	 64% 27% 5% 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
3	CL	C	4	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11032 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 Gentisate 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2714	1727	473	500	14	0	0	0
1	B	348	2701	1719	468	500	14	0	0	0
1	C	348	2699	1718	466	501	14	0	0	0
1	D	352	2728	1735	474	505	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	MET	HIS	engineered mutation	UNP Q67FT0
B	163	MET	HIS	engineered mutation	UNP Q67FT0
C	163	MET	HIS	engineered mutation	UNP Q67FT0
D	163	MET	HIS	engineered mutation	UNP Q67FT0

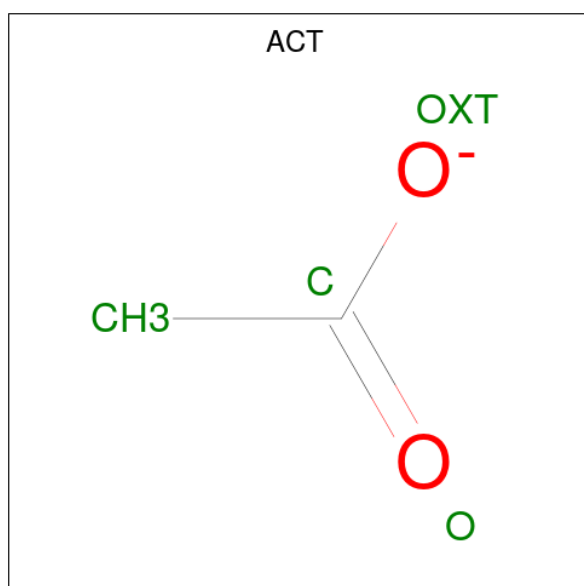
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

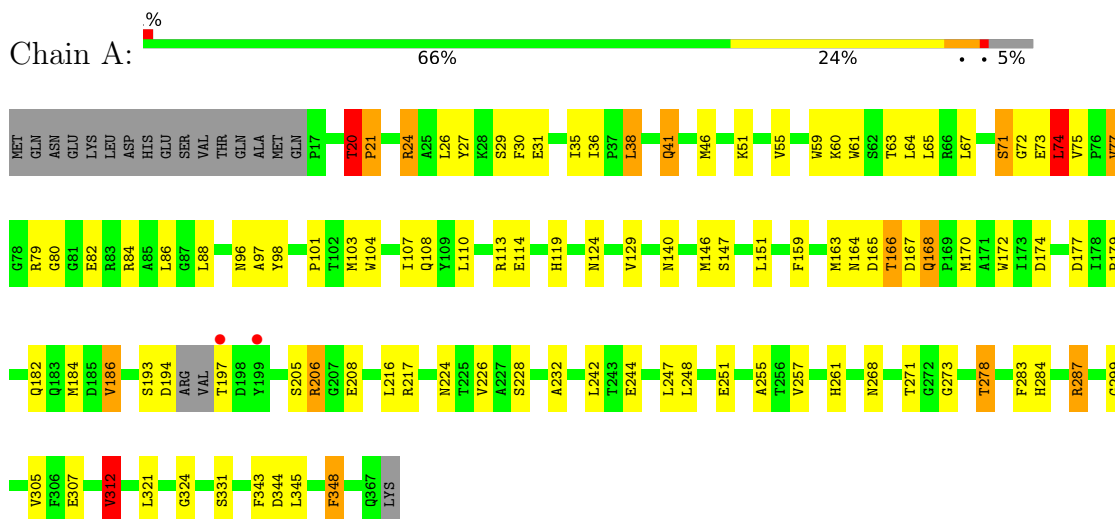
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	49	Total O 49 49	0	0
5	C	62	Total O 62 62	0	0
5	D	30	Total O 30 30	0	0

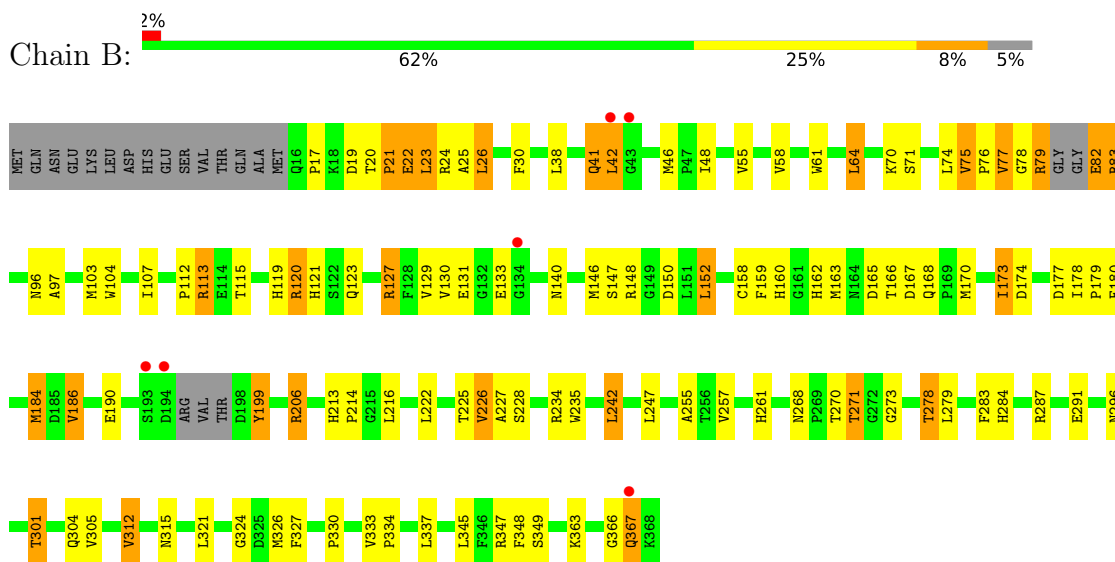
### 3 Residue-property plots [i](#)

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

- Molecule 1: Gentisate 1,2-dioxygenase

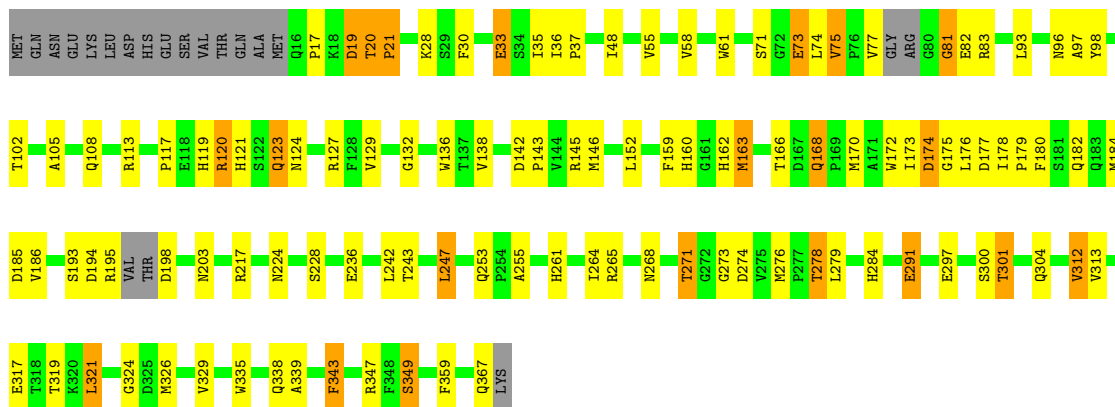


- Molecule 1: Gentisate 1,2-dioxygenase

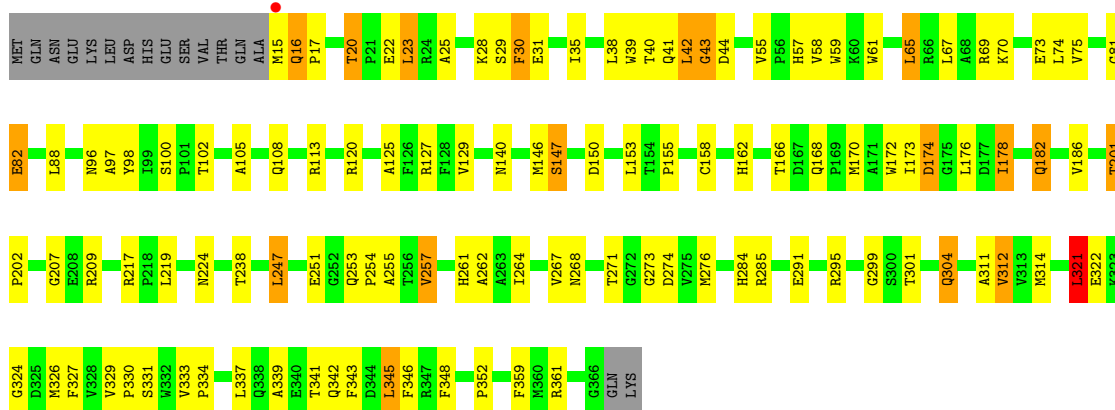


- Molecule 1: Gentisate 1,2-dioxygenase





● Molecule 1: Gentsiate 1,2-dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.02Å 133.02Å 190.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 109.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.90) 98.2 (109.11-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.262 0.197 , 0.262	Depositor DCC
$R_{free}$ test set	1894 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CL, ACT

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	0.78	0/2793	0.82	1/3804 (0.0%)
1	B	0.76	1/2777 (0.0%)	0.86	2/3781 (0.1%)
1	C	0.77	0/2775	0.84	1/3779 (0.0%)
1	D	0.74	0/2808	0.81	2/3831 (0.1%)
All	All	0.76	1/11153 (0.0%)	0.83	6/15195 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	CYS	CB-SG	-5.96	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	VAL	CB-CA-C	-7.71	96.75	111.40
1	B	127	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	D	257	VAL	CB-CA-C	-5.79	100.40	111.40
1	D	321	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	64	LEU	CA-CB-CG	5.66	128.32	115.30
1	C	312	VAL	CB-CA-C	-5.28	101.36	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	GLY	Peptide

## 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	2714	0	2591	102	0
1	B	2701	0	2555	101	0
1	C	2699	0	2562	97	0
1	D	2728	0	2588	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	2	0
3	D	1	0	0	0	0
4	A	4	0	3	0	0
4	D	4	0	3	0	0
5	A	33	0	0	4	0
5	B	49	0	0	3	0
5	C	62	0	0	7	0
5	D	30	0	0	5	0
All	All	11032	0	10302	372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:CE	1:C:102:THR:HG22	1.63	1.26
1:A:168:GLN:HB2	5:A:402:HOH:O	1.40	1.21
1:A:20:THR:H	1:A:21:PRO:HD2	1.03	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE1	1:C:102:THR:HG22	1.25	1.12
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.11	1.08
1:D:312:VAL:HG22	1:D:321:LEU:HD21	1.27	1.08
1:B:38:LEU:O	1:B:41:GLN:HB2	1.55	1.06
1:C:301:THR:HG21	1:C:347:ARG:HE	1.14	1.05
1:A:184:MET:HE3	1:C:102:THR:CG2	1.90	1.01
1:B:271:THR:HG22	1:B:273:GLY:H	1.27	0.98
1:A:184:MET:HE3	1:C:102:THR:HG22	1.43	0.97
1:C:271:THR:HG22	1:C:273:GLY:H	1.30	0.97
1:D:166:THR:HG22	1:D:168:GLN:H	1.30	0.97
1:B:166:THR:HG22	1:B:168:GLN:H	1.32	0.95
1:C:123:GLN:H	1:C:123:GLN:HE21	1.08	0.94
1:A:257:VAL:HG21	1:D:219:LEU:HB2	1.50	0.93
1:A:184:MET:CE	1:C:102:THR:CG2	2.45	0.93
1:A:63:THR:HG21	1:C:33:GLU:HG2	1.52	0.92
1:A:206:ARG:HH11	1:A:206:ARG:CG	1.82	0.92
1:A:20:THR:N	1:A:21:PRO:HD2	1.85	0.91
1:B:103:MET:CE	1:B:348:PHE:CD2	2.54	0.91
1:C:98:TYR:OH	1:C:182:GLN:NE2	2.05	0.89
1:B:177:ASP:OD2	1:B:278:THR:HG21	1.73	0.88
1:A:206:ARG:HG2	1:A:206:ARG:NH1	1.80	0.87
1:D:42:LEU:O	1:D:44:ASP:N	2.07	0.87
1:B:206:ARG:HD3	1:C:253:GLN:NE2	1.90	0.86
1:B:79:ARG:C	1:B:83:ARG:H	1.79	0.85
1:C:166:THR:HG22	1:C:168:GLN:H	1.39	0.85
1:D:153:LEU:HD22	1:D:276:MET:CE	2.07	0.85
1:C:177:ASP:OD2	1:C:278:THR:HG21	1.77	0.84
1:A:73:GLU:O	1:A:74:LEU:HD12	1.77	0.84
1:D:153:LEU:HD22	1:D:276:MET:HE2	1.59	0.83
1:D:217:ARG:HH22	1:D:224:ASN:HD22	1.25	0.83
1:C:301:THR:CG2	1:C:347:ARG:HE	1.92	0.82
1:A:84:ARG:NH2	1:A:114:GLU:OE1	2.13	0.82
1:B:103:MET:HE1	1:B:348:PHE:CD2	2.15	0.82
1:C:217:ARG:HH22	1:C:224:ASN:ND2	1.77	0.81
1:D:16:GLN:H	1:D:17:PRO:CD	1.93	0.81
1:A:217:ARG:HH22	1:A:224:ASN:HD22	1.28	0.81
1:B:184:MET:HE1	1:D:102:THR:HG22	1.62	0.81
1:D:170:MET:HE3	1:D:172:TRP:HE3	1.44	0.81
1:D:127:ARG:HH12	1:D:162:HIS:HD2	1.26	0.81
1:A:257:VAL:CG2	1:D:219:LEU:HB2	2.11	0.80
1:B:261:HIS:NE2	1:B:284:HIS:HD2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:GLN:HB2	1:D:326:MET:HG2	1.63	0.79
3:A:1:CL:CL	5:A:376:HOH:O	2.38	0.79
1:A:20:THR:H	1:A:21:PRO:CD	1.90	0.78
1:D:127:ARG:HH12	1:D:162:HIS:CD2	2.01	0.78
1:A:305:VAL:HA	1:A:345:LEU:CD1	2.14	0.77
1:D:16:GLN:H	1:D:17:PRO:HD2	1.48	0.77
1:A:206:ARG:HH21	1:D:254:PRO:HG2	1.49	0.76
1:A:217:ARG:HH22	1:A:224:ASN:ND2	1.83	0.76
1:A:177:ASP:OD2	1:A:278:THR:HG21	1.84	0.75
1:D:81:GLY:O	1:D:82:GLU:CB	2.34	0.75
1:A:261:HIS:NE2	1:A:284:HIS:HD2	1.84	0.75
1:C:163:MET:O	1:C:163:MET:HG2	1.86	0.75
1:D:341:THR:HG22	1:D:342:GLN:H	1.53	0.74
1:D:20:THR:HG22	1:D:23:LEU:H	1.51	0.73
1:B:301:THR:HG21	1:B:347:ARG:NE	2.03	0.73
1:C:301:THR:HG21	1:C:347:ARG:NE	1.98	0.72
1:A:98:TYR:OH	1:A:182:GLN:NE2	2.23	0.71
1:C:77:VAL:HG21	5:C:429:HOH:O	1.88	0.71
1:D:15:MET:N	1:D:40:THR:HA	2.05	0.71
1:B:184:MET:CE	1:D:102:THR:HG22	2.20	0.71
1:C:349:SER:HB3	5:C:377:HOH:O	1.91	0.70
1:B:46:MET:CE	1:D:178:ILE:HD11	2.21	0.70
1:C:193:SER:HA	5:C:409:HOH:O	1.90	0.70
1:D:155:PRO:HG2	1:D:158:CYS:SG	2.31	0.70
1:D:96:ASN:O	1:D:97:ALA:HB3	1.92	0.70
1:D:312:VAL:HG22	1:D:321:LEU:CD2	2.14	0.70
1:B:96:ASN:O	1:B:97:ALA:HB3	1.92	0.70
1:B:103:MET:CE	1:B:348:PHE:HD2	2.04	0.70
1:C:75:VAL:HG22	1:C:81:GLY:HA2	1.74	0.70
1:C:261:HIS:NE2	1:C:284:HIS:HD2	1.90	0.69
1:C:271:THR:HG22	1:C:273:GLY:N	2.05	0.69
1:D:43:GLY:HA2	5:D:381:HOH:O	1.92	0.69
1:C:123:GLN:HE21	1:C:123:GLN:N	1.88	0.68
1:C:117:PRO:O	5:C:404:HOH:O	2.11	0.68
1:D:304:GLN:CB	1:D:326:MET:HG2	2.23	0.68
1:C:20:THR:HG22	1:C:21:PRO:N	2.08	0.68
1:D:98:TYR:OH	1:D:182:GLN:NE2	2.27	0.68
1:C:123:GLN:H	1:C:123:GLN:NE2	1.89	0.68
1:C:98:TYR:HH	1:C:182:GLN:HE21	1.42	0.67
1:C:291:GLU:HG3	1:C:338:GLN:HG2	1.75	0.67
1:D:170:MET:HE3	1:D:172:TRP:CE3	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:O	1:A:31:GLU:HG3	1.95	0.67
1:A:166:THR:HG23	1:A:168:GLN:H	1.60	0.67
1:A:166:THR:CG2	1:A:168:GLN:H	2.08	0.67
1:B:41:GLN:HA	1:B:41:GLN:OE1	1.95	0.66
1:B:216:LEU:HD22	1:C:264:ILE:HD13	1.77	0.66
1:B:271:THR:HG22	1:B:273:GLY:N	2.06	0.66
1:A:271:THR:HG22	1:A:273:GLY:H	1.60	0.66
1:D:75:VAL:HG12	1:D:81:GLY:N	2.11	0.66
1:A:184:MET:HE2	1:C:180:PHE:HD2	1.61	0.66
1:D:341:THR:HG22	1:D:342:GLN:N	2.11	0.66
1:B:77:VAL:CB	5:B:407:HOH:O	2.43	0.66
1:D:170:MET:CE	1:D:172:TRP:CE3	2.79	0.66
1:C:75:VAL:CG2	1:C:81:GLY:HA2	2.26	0.65
1:D:81:GLY:O	1:D:82:GLU:HB2	1.96	0.65
1:D:271:THR:HG22	1:D:273:GLY:H	1.60	0.65
1:D:311:ALA:HA	1:D:321:LEU:HD22	1.78	0.65
1:A:312:VAL:HG22	1:A:321:LEU:HD21	1.78	0.65
1:A:206:ARG:HH21	1:D:254:PRO:CG	2.09	0.65
1:C:349:SER:CB	5:C:377:HOH:O	2.45	0.64
1:B:312:VAL:HG13	1:B:337:LEU:HD23	1.80	0.63
1:D:16:GLN:N	1:D:17:PRO:CD	2.60	0.63
1:D:166:THR:HG22	1:D:168:GLN:N	2.10	0.63
1:D:247:LEU:O	1:D:251:GLU:HG3	1.99	0.63
1:B:127:ARG:HH12	1:B:162:HIS:CD2	2.15	0.62
1:B:184:MET:CE	1:D:102:THR:CG2	2.77	0.62
1:A:86:LEU:HD13	1:C:35:ILE:HG21	1.82	0.62
1:C:19:ASP:OD2	1:C:19:ASP:N	2.32	0.62
1:C:132:GLY:HA3	1:C:170:MET:HG3	1.80	0.62
1:B:103:MET:HE3	1:B:348:PHE:CD2	2.34	0.62
1:B:301:THR:CG2	1:B:349:SER:HB3	2.30	0.62
1:A:63:THR:CG2	1:C:33:GLU:HG2	2.28	0.61
1:C:217:ARG:HH22	1:C:224:ASN:HD22	1.47	0.61
1:D:38:LEU:O	1:D:41:GLN:HB2	2.00	0.61
1:B:107:ILE:CD1	1:B:173:ILE:HG22	2.29	0.61
1:B:127:ARG:NH2	1:B:160:HIS:HD2	1.99	0.61
1:B:107:ILE:HD12	1:B:173:ILE:HG22	1.82	0.61
1:A:108:GLN:HG2	1:A:172:TRP:CE2	2.36	0.61
1:B:226:VAL:HG23	5:B:394:HOH:O	2.01	0.61
1:D:166:THR:CG2	1:D:168:GLN:H	2.10	0.61
1:C:108:GLN:HG2	1:C:172:TRP:CZ2	2.35	0.60
1:B:127:ARG:HH12	1:B:162:HIS:HD2	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:THR:CG2	1:B:279:LEU:HG	2.32	0.60
3:C:4:CL:CL	5:C:414:HOH:O	2.52	0.60
1:B:166:THR:HG22	1:B:167:ASP:N	2.17	0.59
1:B:184:MET:HE2	1:D:102:THR:CG2	2.32	0.59
1:A:216:LEU:HD22	1:D:264:ILE:HD13	1.83	0.59
1:B:46:MET:HE2	1:D:178:ILE:HD11	1.85	0.58
1:B:180:PHE:O	1:B:184:MET:HB2	2.04	0.58
1:B:225:THR:HG22	1:B:270:THR:OG1	2.02	0.58
1:B:103:MET:CE	1:B:348:PHE:CE2	2.86	0.57
1:D:274:ASP:OD2	1:D:352:PRO:HG3	2.04	0.57
1:A:103:MET:HE1	1:A:348:PHE:CD2	2.40	0.57
1:B:103:MET:HE3	1:B:348:PHE:HD2	1.65	0.57
1:B:120:ARG:NH2	1:B:190:GLU:OE1	2.37	0.57
1:D:312:VAL:HG11	1:D:327:PHE:CE1	2.40	0.57
1:B:301:THR:HG21	1:B:347:ARG:HE	1.68	0.57
1:C:173:ILE:HD11	1:C:304:GLN:HG3	1.85	0.57
1:A:184:MET:CE	1:C:180:PHE:HD2	2.17	0.56
1:B:304:GLN:HG2	1:B:326:MET:HG2	1.86	0.56
1:B:113:ARG:HG2	1:B:166:THR:O	2.06	0.56
1:C:304:GLN:HG2	1:C:326:MET:HG2	1.87	0.56
1:B:96:ASN:O	1:B:97:ALA:CB	2.54	0.56
1:D:299:GLY:O	1:D:331:SER:HA	2.06	0.56
1:A:96:ASN:O	1:A:97:ALA:HB3	2.06	0.55
1:A:20:THR:N	1:A:21:PRO:CD	2.59	0.55
1:B:82:GLU:O	1:B:83:ARG:CB	2.55	0.55
1:A:287:ARG:HH11	1:A:287:ARG:CG	2.19	0.55
1:C:71:SER:O	1:C:75:VAL:HG13	2.07	0.55
1:A:194:ASP:O	1:A:197:THR:N	2.40	0.55
1:A:98:TYR:CD1	1:A:179:PRO:HG3	2.41	0.55
1:B:301:THR:HG22	1:B:349:SER:HB3	1.87	0.55
1:A:251:GLU:CD	1:D:209:ARG:HH22	2.10	0.55
1:C:127:ARG:HH12	1:C:162:HIS:CD2	2.25	0.55
1:C:166:THR:HG22	1:C:168:GLN:HB2	1.88	0.55
1:C:291:GLU:CG	1:C:338:GLN:HG2	2.36	0.55
1:A:184:MET:HE2	1:C:180:PHE:CD2	2.41	0.54
1:B:366:GLY:O	1:B:367:GLN:HB2	2.07	0.54
1:B:166:THR:HG22	1:B:168:GLN:N	2.13	0.54
1:D:108:GLN:HG2	1:D:172:TRP:CZ2	2.43	0.54
1:D:201:THR:O	1:D:201:THR:HG23	2.07	0.54
1:D:207:GLY:HA3	5:D:386:HOH:O	2.07	0.54
1:A:299:GLY:O	1:A:331:SER:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:HB3	5:C:402:HOH:O	2.08	0.53
1:A:101:PRO:HG2	1:C:185:ASP:OD2	2.07	0.53
1:A:108:GLN:HG2	1:A:172:TRP:CZ2	2.43	0.53
1:B:23:LEU:O	1:B:26:LEU:N	2.40	0.53
1:C:217:ARG:NH2	1:C:224:ASN:ND2	2.51	0.53
1:D:202:PRO:HA	5:D:389:HOH:O	2.09	0.53
1:D:217:ARG:HH22	1:D:224:ASN:ND2	2.01	0.53
1:C:166:THR:HG22	1:C:168:GLN:N	2.18	0.53
1:C:120:ARG:HB2	1:C:159:PHE:CD2	2.43	0.52
1:C:166:THR:CG2	1:C:168:GLN:HB2	2.38	0.52
1:A:305:VAL:HA	1:A:345:LEU:HD13	1.91	0.52
1:B:127:ARG:NH2	1:B:160:HIS:CD2	2.76	0.52
1:C:195:ARG:O	1:C:198:ASP:N	2.43	0.52
1:B:186:VAL:HG22	1:D:359:PHE:HB3	1.92	0.52
1:A:63:THR:HG21	1:C:33:GLU:CG	2.32	0.52
1:D:30:PHE:HB3	1:D:35:ILE:O	2.10	0.52
1:B:287:ARG:NH1	1:B:287:ARG:HG3	2.26	0.51
1:A:217:ARG:NH2	1:A:224:ASN:HD22	2.03	0.51
1:A:104:TRP:HZ3	1:A:174:ASP:HB3	1.75	0.51
1:B:228:SER:HB2	1:B:268:ASN:HA	1.92	0.51
1:D:345:LEU:N	1:D:345:LEU:HD22	2.27	0.50
1:A:59:TRP:CD2	1:A:88:LEU:HD23	2.46	0.50
1:A:103:MET:CE	1:A:348:PHE:CD2	2.94	0.50
1:D:25:ALA:O	1:D:28:LYS:HB3	2.12	0.50
1:C:96:ASN:O	1:C:97:ALA:HB3	2.11	0.50
1:D:42:LEU:C	1:D:44:ASP:H	2.12	0.50
1:C:108:GLN:HG2	1:C:172:TRP:CE2	2.47	0.50
1:C:175:GLY:C	1:C:176:LEU:HD12	2.32	0.50
1:C:313:VAL:CG2	1:C:338:GLN:HE22	2.25	0.50
1:B:312:VAL:HG11	1:B:327:PHE:CE2	2.47	0.49
1:C:278:THR:CG2	1:C:279:LEU:HG	2.43	0.49
1:A:228:SER:HB2	1:A:268:ASN:HA	1.93	0.49
1:B:127:ARG:NH1	1:B:162:HIS:CD2	2.81	0.49
1:B:127:ARG:NH1	1:B:162:HIS:HD2	2.09	0.49
1:C:228:SER:HB2	1:C:268:ASN:HA	1.94	0.49
1:A:146:MET:SD	1:A:170:MET:HE1	2.52	0.49
1:B:301:THR:HG23	1:B:349:SER:HB3	1.95	0.49
1:C:312:VAL:HG22	1:C:321:LEU:HD21	1.94	0.48
1:C:265:ARG:HD3	1:C:274:ASP:OD1	2.14	0.48
1:A:71:SER:O	1:A:84:ARG:HD2	2.13	0.48
1:B:127:ARG:HH21	1:B:160:HIS:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ASN:O	1:D:97:ALA:CB	2.55	0.48
1:D:58:VAL:HG12	1:D:327:PHE:HB3	1.96	0.48
1:D:271:THR:HG22	1:D:273:GLY:N	2.27	0.48
1:A:103:MET:CE	1:A:348:PHE:HD2	2.27	0.48
1:D:61:TRP:HB2	1:D:324:GLY:C	2.33	0.48
1:D:81:GLY:O	1:D:82:GLU:HB3	2.11	0.48
1:D:82:GLU:OE1	1:D:82:GLU:HA	2.13	0.48
1:D:147:SER:HB2	1:D:150:ASP:OD2	2.14	0.48
1:B:140:ASN:HD21	1:B:159:PHE:H	1.62	0.47
1:C:98:TYR:CD2	1:C:179:PRO:HB3	2.49	0.47
1:C:236:GLU:CD	1:C:236:GLU:H	2.17	0.47
1:D:108:GLN:HG2	1:D:172:TRP:CE2	2.48	0.47
1:D:170:MET:CE	1:D:172:TRP:HE3	2.15	0.47
1:A:36:ILE:HD12	1:C:97:ALA:HB2	1.96	0.47
1:A:206:ARG:CG	1:A:206:ARG:NH1	2.52	0.47
1:B:150:ASP:OD2	1:B:234:ARG:NH1	2.47	0.47
1:D:125:ALA:HB2	1:D:176:LEU:HG	1.96	0.47
1:A:287:ARG:NH1	1:A:287:ARG:HG3	2.29	0.47
1:B:129:VAL:HG21	1:B:146:MET:HB3	1.96	0.47
1:B:278:THR:HG22	1:B:279:LEU:HG	1.95	0.47
1:B:312:VAL:HG13	1:B:337:LEU:CD2	2.44	0.47
1:B:330:PRO:HG2	1:B:333:VAL:HG21	1.95	0.47
1:D:127:ARG:NH1	1:D:162:HIS:CD2	2.79	0.47
1:D:262:ALA:HB3	1:D:285:ARG:HB3	1.95	0.47
1:A:193:SER:N	1:A:194:ASP:HB2	2.30	0.47
1:A:186:VAL:HG22	1:C:359:PHE:HB3	1.96	0.47
1:A:206:ARG:HB3	5:D:377:HOH:O	2.15	0.47
1:B:184:MET:HE2	1:D:102:THR:HG23	1.96	0.47
1:B:75:VAL:HA	1:B:76:PRO:HD3	1.87	0.47
1:D:125:ALA:CB	1:D:176:LEU:HG	2.45	0.47
1:B:140:ASN:ND2	1:B:159:PHE:H	2.13	0.47
1:C:312:VAL:CG2	1:C:321:LEU:HD21	2.44	0.47
1:D:312:VAL:HG13	1:D:337:LEU:HD23	1.97	0.47
1:B:119:HIS:CD2	1:B:121:HIS:CD2	3.03	0.47
1:B:199:TYR:N	1:B:199:TYR:CD2	2.83	0.47
1:D:253:GLN:NE2	5:D:377:HOH:O	2.37	0.47
1:B:278:THR:HG23	1:B:279:LEU:HG	1.97	0.46
1:B:261:HIS:NE2	1:B:284:HIS:CD2	2.71	0.46
1:C:61:TRP:HB2	1:C:324:GLY:C	2.34	0.46
1:D:173:ILE:CD1	1:D:304:GLN:HG2	2.44	0.46
1:B:287:ARG:HG3	1:B:287:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:THR:HG22	1:D:22:GLU:N	2.30	0.46
1:A:124:ASN:HD22	1:A:278:THR:HG21	1.81	0.46
1:A:140:ASN:ND2	1:A:159:PHE:H	2.14	0.46
1:D:129:VAL:HG21	1:D:146:MET:HB3	1.96	0.46
1:B:166:THR:CG2	1:B:167:ASP:N	2.79	0.46
1:B:242:LEU:HD21	1:B:283:PHE:HD2	1.81	0.46
1:C:124:ASN:HB3	1:C:276:MET:SD	2.56	0.46
1:A:38:LEU:HD13	1:C:83:ARG:HB3	1.98	0.46
1:B:23:LEU:C	1:B:25:ALA:N	2.69	0.46
1:D:264:ILE:C	1:D:264:ILE:HD12	2.36	0.46
1:D:330:PRO:HG2	1:D:333:VAL:HG21	1.97	0.46
1:C:73:GLU:O	1:C:74:LEU:HB2	2.16	0.46
1:B:104:TRP:HZ3	1:B:174:ASP:HB2	1.81	0.45
1:B:112:PRO:HB3	1:B:167:ASP:O	2.16	0.45
1:D:268:ASN:C	1:D:268:ASN:OD1	2.55	0.45
1:D:65:LEU:O	1:D:69:ARG:HG3	2.16	0.45
1:A:30:PHE:HB3	1:A:35:ILE:O	2.17	0.45
1:B:79:ARG:NH2	5:B:407:HOH:O	2.49	0.45
1:A:124:ASN:ND2	1:A:278:THR:CG2	2.79	0.45
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.85	0.45
1:D:346:PHE:CE2	1:D:348:PHE:CD1	3.05	0.45
1:D:170:MET:HE2	1:D:172:TRP:CE3	2.51	0.45
1:C:145:ARG:NH1	1:C:203:ASN:O	2.45	0.45
1:D:57:HIS:CD2	1:D:58:VAL:O	2.69	0.45
1:D:73:GLU:HB3	1:D:74:LEU:HD13	1.98	0.45
1:D:201:THR:N	1:D:202:PRO:HD3	2.31	0.45
1:D:295:ARG:O	1:D:334:PRO:HA	2.16	0.45
1:D:312:VAL:HG11	1:D:327:PHE:CZ	2.52	0.45
1:A:271:THR:HG22	1:A:273:GLY:N	2.29	0.45
1:B:178:ILE:HB	1:B:179:PRO:HD3	1.99	0.45
1:B:127:ARG:HB2	1:B:152:LEU:HB2	1.99	0.44
1:B:235:TRP:HZ3	1:B:283:PHE:CZ	2.35	0.44
1:C:217:ARG:NH2	1:C:224:ASN:HD22	2.13	0.44
1:D:59:TRP:CE3	1:D:88:LEU:HD23	2.51	0.44
1:C:93:LEU:O	1:C:96:ASN:HB2	2.18	0.44
1:B:184:MET:CE	1:B:184:MET:HA	2.46	0.44
1:C:119:HIS:CD2	1:C:121:HIS:CD2	3.05	0.44
1:D:261:HIS:NE2	1:D:284:HIS:HD2	2.15	0.44
1:C:142:ASP:HA	1:C:143:PRO:HD3	1.86	0.44
1:A:193:SER:CA	1:A:194:ASP:HB2	2.47	0.44
1:A:283:PHE:HE2	1:A:344:ASP:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TRP:CE3	1:A:88:LEU:HD23	2.53	0.43
1:C:129:VAL:HG21	1:C:146:MET:HB3	2.00	0.43
1:A:312:VAL:CG2	1:A:321:LEU:HD11	2.48	0.43
1:A:20:THR:HG23	1:A:24:ARG:NH1	2.33	0.43
1:D:201:THR:O	1:D:201:THR:CG2	2.66	0.43
1:A:140:ASN:HD21	1:A:159:PHE:H	1.67	0.43
1:C:304:GLN:CG	1:C:326:MET:HG2	2.47	0.43
1:D:30:PHE:O	1:D:31:GLU:C	2.57	0.43
1:C:71:SER:O	1:C:75:VAL:CG1	2.67	0.43
1:C:297:GLU:OE2	3:C:4:CL:CL	2.74	0.43
1:B:113:ARG:NH1	1:B:167:ASP:OD1	2.51	0.43
1:D:170:MET:HE2	1:D:172:TRP:CZ3	2.54	0.43
1:A:312:VAL:HG22	1:A:321:LEU:CD2	2.48	0.43
1:D:105:ALA:HA	1:D:174:ASP:O	2.19	0.43
1:B:61:TRP:HB2	1:B:324:GLY:C	2.39	0.42
1:A:205:SER:OG	1:A:208:GLU:HG3	2.19	0.42
1:B:30:PHE:HE1	1:D:67:LEU:HB3	1.84	0.42
1:D:301:THR:HG22	1:D:329:VAL:HB	2.00	0.42
1:B:121:HIS:HB2	1:B:123:GLN:OE1	2.19	0.42
1:B:366:GLY:O	1:B:367:GLN:CB	2.67	0.42
1:C:329:VAL:HG11	1:C:335:TRP:CD1	2.54	0.42
1:D:67:LEU:N	1:D:67:LEU:HD23	2.32	0.42
1:A:251:GLU:OE2	1:D:209:ARG:NH2	2.49	0.42
1:C:105:ALA:HA	1:C:174:ASP:O	2.18	0.42
1:A:61:TRP:HB2	1:A:324:GLY:C	2.40	0.42
1:A:216:LEU:HD11	1:D:238:THR:HA	2.02	0.42
1:A:268:ASN:C	1:A:268:ASN:OD1	2.56	0.42
1:B:38:LEU:O	1:B:41:GLN:CB	2.46	0.42
1:A:177:ASP:OD2	1:A:278:THR:CG2	2.62	0.42
1:A:113:ARG:NH1	1:A:167:ASP:OD1	2.53	0.42
1:A:244:GLU:HG3	1:D:209:ARG:HB3	2.01	0.42
1:B:242:LEU:HD21	1:B:283:PHE:CD2	2.54	0.42
1:C:20:THR:CG2	1:C:21:PRO:N	2.78	0.42
1:C:178:ILE:HB	1:C:179:PRO:HD3	2.02	0.42
1:C:313:VAL:HG23	1:C:338:GLN:NE2	2.35	0.42
1:A:166:THR:HG22	1:A:168:GLN:H	1.83	0.42
1:B:225:THR:HG23	1:B:227:ALA:O	2.20	0.42
1:A:103:MET:HE2	1:A:348:PHE:HD2	1.85	0.42
1:A:77:VAL:HG12	1:A:82:GLU:HG3	2.03	0.41
1:B:213:HIS:HA	1:B:214:PRO:HD2	1.89	0.41
1:A:110:LEU:HD21	1:A:164:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:HD22	1:A:140:ASN:HA	1.75	0.41
5:A:376:HOH:O	1:D:219:LEU:HD13	2.20	0.41
1:B:19:ASP:O	1:B:21:PRO:N	2.53	0.41
1:B:199:TYR:N	1:B:199:TYR:HD2	2.18	0.41
1:B:70:LYS:HD2	1:B:70:LYS:HA	1.78	0.41
1:C:339:ALA:HB1	1:C:343:PHE:HB2	2.03	0.41
1:C:19:ASP:O	1:C:20:THR:O	2.38	0.41
1:C:136:TRP:HB2	1:C:163:MET:SD	2.61	0.41
1:C:261:HIS:NE2	1:C:284:HIS:CD2	2.79	0.41
1:B:146:MET:HB2	1:B:170:MET:HE1	2.01	0.41
1:A:348:PHE:CD1	1:A:348:PHE:N	2.89	0.41
1:B:130:VAL:O	1:B:148:ARG:NH1	2.50	0.41
1:C:170:MET:CE	1:C:172:TRP:CE3	3.04	0.41
1:D:339:ALA:HB1	1:D:343:PHE:HB2	2.02	0.41
1:A:104:TRP:HZ3	1:A:174:ASP:CB	2.33	0.41
1:A:110:LEU:CD2	1:A:164:ASN:HB2	2.51	0.41
1:A:129:VAL:HB	1:A:147:SER:O	2.21	0.41
1:C:278:THR:HG23	1:C:279:LEU:HG	2.01	0.41
1:D:346:PHE:HE2	1:D:348:PHE:CD1	2.38	0.41
1:A:38:LEU:O	1:A:41:GLN:HB2	2.21	0.41
1:A:64:LEU:HD13	1:A:107:ILE:HD11	2.03	0.41
1:A:129:VAL:HG22	1:A:146:MET:HE2	2.03	0.41
1:B:75:VAL:HG11	1:D:39:TRP:CZ2	2.56	0.41
1:C:138:VAL:O	1:C:160:HIS:HA	2.21	0.41
1:C:313:VAL:CG2	1:C:338:GLN:NE2	2.85	0.41
1:D:314:MET:CE	1:D:327:PHE:CD1	3.04	0.41
1:A:151:LEU:O	1:A:232:ALA:HA	2.21	0.40
1:A:166:THR:HG23	5:A:402:HOH:O	2.19	0.40
1:B:71:SER:O	1:B:75:VAL:HG13	2.20	0.40
1:B:315:ASN:ND2	1:B:334:PRO:HD2	2.36	0.40
1:C:243:THR:HG22	1:C:247:LEU:HD22	2.03	0.40
1:D:346:PHE:CE2	1:D:348:PHE:HD1	2.39	0.40
1:B:76:PRO:C	1:B:78:GLY:H	2.25	0.40
1:B:305:VAL:HA	1:B:345:LEU:HD13	2.03	0.40
1:C:36:ILE:HA	1:C:37:PRO:HD2	1.96	0.40
1:C:184:MET:O	1:C:185:ASP:HB2	2.21	0.40
1:B:296:ASN:HB2	1:B:363:LYS:HB3	2.04	0.40
1:D:38:LEU:O	1:D:38:LEU:HG	2.20	0.40
1:A:67:LEU:HD13	1:C:30:PHE:CD1	2.56	0.40
1:A:104:TRP:CZ3	1:A:174:ASP:HB3	2.56	0.40
1:A:261:HIS:NE2	1:A:284:HIS:CD2	2.76	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	345/368 (94%)	316 (92%)	21 (6%)	8 (2%)	6	23
1	B	342/368 (93%)	318 (93%)	14 (4%)	10 (3%)	4	18
1	C	342/368 (93%)	321 (94%)	15 (4%)	6 (2%)	8	29
1	D	350/368 (95%)	325 (93%)	19 (5%)	6 (2%)	9	31
All	All	1379/1472 (94%)	1280 (93%)	69 (5%)	30 (2%)	6	24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	B	20	THR
1	B	22	GLU
1	B	42	LEU
1	B	83	ARG
1	B	367	GLN
1	C	17	PRO
1	C	20	THR
1	C	21	PRO
1	D	16	GLN
1	D	43	GLY
1	A	79	ARG
1	A	255	ALA
1	B	21	PRO
1	C	82	GLU
1	C	255	ALA
1	D	42	LEU
1	D	82	GLU
1	D	255	ALA
1	A	21	PRO

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Mol	Chain	Res	Type
1	A	74	LEU
1	B	24	ARG
1	B	255	ALA
1	A	72	GLY
1	B	17	PRO
1	A	71	SER
1	B	77	VAL
1	D	30	PHE
1	A	26	LEU
1	C	81	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	282/307 (92%)	253 (90%)	29 (10%)	7	22
1	B	277/307 (90%)	239 (86%)	38 (14%)	3	11
1	C	279/307 (91%)	249 (89%)	30 (11%)	6	20
1	D	281/307 (92%)	255 (91%)	26 (9%)	9	27
All	All	1119/1228 (91%)	996 (89%)	123 (11%)	6	19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	24	ARG
1	A	29	SER
1	A	38	LEU
1	A	41	GLN
1	A	46	MET
1	A	51	LYS
1	A	55	VAL
1	A	60	LYS
1	A	65	LEU
1	A	74	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	75	VAL
1	A	77	VAL
1	A	119	HIS
1	A	163	MET
1	A	165	ASP
1	A	166	THR
1	A	168	GLN
1	A	186	VAL
1	A	206	ARG
1	A	226	VAL
1	A	242	LEU
1	A	247	LEU
1	A	278	THR
1	A	287	ARG
1	A	307	GLU
1	A	312	VAL
1	A	343	PHE
1	A	348	PHE
1	B	22	GLU
1	B	23	LEU
1	B	26	LEU
1	B	41	GLN
1	B	42	LEU
1	B	48	ILE
1	B	55	VAL
1	B	58	VAL
1	B	64	LEU
1	B	74	LEU
1	B	75	VAL
1	B	79	ARG
1	B	82	GLU
1	B	113	ARG
1	B	115	THR
1	B	120	ARG
1	B	131	GLU
1	B	133	GLU
1	B	147	SER
1	B	152	LEU
1	B	163	MET
1	B	165	ASP
1	B	173	ILE
1	B	184	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	186	VAL
1	B	199	TYR
1	B	206	ARG
1	B	222	LEU
1	B	226	VAL
1	B	242	LEU
1	B	247	LEU
1	B	257	VAL
1	B	271	THR
1	B	278	THR
1	B	291	GLU
1	B	301	THR
1	B	312	VAL
1	B	321	LEU
1	C	19	ASP
1	C	28	LYS
1	C	33	GLU
1	C	48	ILE
1	C	55	VAL
1	C	58	VAL
1	C	73	GLU
1	C	75	VAL
1	C	113	ARG
1	C	120	ARG
1	C	123	GLN
1	C	152	LEU
1	C	163	MET
1	C	168	GLN
1	C	174	ASP
1	C	186	VAL
1	C	194	ASP
1	C	242	LEU
1	C	247	LEU
1	C	271	THR
1	C	278	THR
1	C	291	GLU
1	C	300	SER
1	C	301	THR
1	C	317	GLU
1	C	319	THR
1	C	321	LEU
1	C	343	PHE

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Mol	Chain	Res	Type
1	C	349	SER
1	C	367	GLN
1	D	20	THR
1	D	23	LEU
1	D	29	SER
1	D	55	VAL
1	D	65	LEU
1	D	70	LYS
1	D	100	SER
1	D	113	ARG
1	D	120	ARG
1	D	140	ASN
1	D	147	SER
1	D	174	ASP
1	D	178	ILE
1	D	182	GLN
1	D	186	VAL
1	D	201	THR
1	D	247	LEU
1	D	257	VAL
1	D	267	VAL
1	D	291	GLU
1	D	304	GLN
1	D	312	VAL
1	D	321	LEU
1	D	322	GLU
1	D	345	LEU
1	D	361	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	140	ASN
1	A	182	GLN
1	A	224	ASN
1	A	284	HIS
1	A	315	ASN
1	B	140	ASN
1	B	162	HIS
1	B	284	HIS
1	B	315	ASN

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Mol	Chain	Res	Type
1	C	57	HIS
1	C	123	GLN
1	C	140	ASN
1	C	162	HIS
1	C	182	GLN
1	C	224	ASN
1	C	253	GLN
1	C	284	HIS
1	C	315	ASN
1	C	338	GLN
1	D	57	HIS
1	D	162	HIS
1	D	182	GLN
1	D	224	ASN
1	D	284	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	A	371	-	3,3,3	0.93	0	3,3,3	1.64	1 (33%)
4	ACT	D	1	2	3,3,3	1.06	0	3,3,3	1.26	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	371	ACT	OXT-C-O	-2.15	114.14	122.05

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	349/368 (94%)	0.04	2 (0%) 89 89	29, 41, 65, 75	0
1	B	348/368 (94%)	0.16	6 (1%) 70 69	27, 40, 69, 81	0
1	C	348/368 (94%)	0.03	0 100 100	28, 40, 67, 75	0
1	D	352/368 (95%)	0.03	1 (0%) 94 94	29, 40, 61, 70	0
All	All	1397/1472 (94%)	0.06	9 (0%) 89 89	27, 40, 65, 81	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	SER	3.9
1	B	194	ASP	2.9
1	B	134	GLY	2.6
1	D	15	MET	2.5
1	B	43	GLY	2.3
1	B	367	GLN	2.2
1	A	199	TYR	2.1
1	A	197	THR	2.1
1	B	42	LEU	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 monosaccharides 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
4	ACT	D	1	4/4	0.88	0.25	53,53,54,54	0
4	ACT	A	371	4/4	0.92	0.14	42,42,42,43	0
3	CL	B	2	1/1	0.96	0.15	32,32,32,32	0
3	CL	C	4	1/1	0.97	0.23	50,50,50,50	0
3	CL	D	3	1/1	0.97	0.13	48,48,48,48	0
3	CL	A	1	1/1	0.97	0.12	42,42,42,42	0
2	FE	D	370	1/1	0.97	0.16	31,31,31,31	0
2	FE	C	370	1/1	0.98	0.13	35,35,35,35	0
2	FE	A	370	1/1	0.98	0.17	40,40,40,40	0
2	FE	B	370	1/1	0.99	0.14	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.