



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:34 am BST

PDB ID : 4KER  
Title : Crystal structure of SsoPox W263V  
Authors : Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.  
Deposited on : 2013-04-26  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

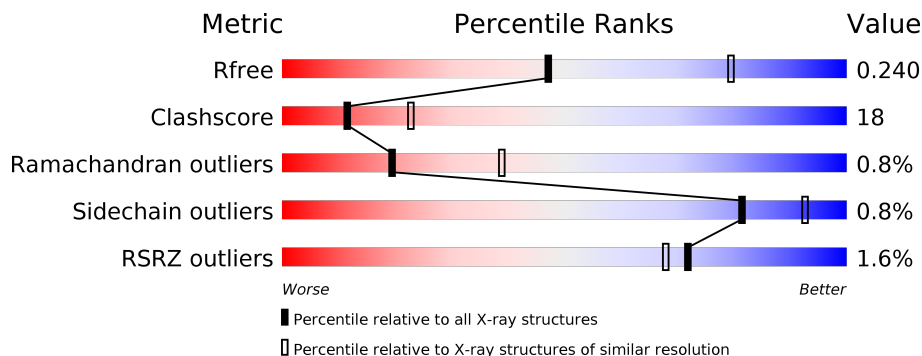
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	314	 2% 69% 30%
1	B	314	 71% 28%
1	C	314	 2% 68% 31%
1	D	314	 3% 68% 31%

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 crite-

ria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	EDO	B	403	-	-	-	X
5	GOL	D	404	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10511 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 Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2517	1615	426	469	7	0	1	0
1	B	314	2506	1606	425	468	7	0	0	0
1	C	314	2506	1606	425	468	7	0	0	0
1	D	314	2514	1611	428	468	7	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	VAL	TRP	ENGINEERED MUTATION	UNP Q97VT7
B	263	VAL	TRP	ENGINEERED MUTATION	UNP Q97VT7
C	263	VAL	TRP	ENGINEERED MUTATION	UNP Q97VT7
D	263	VAL	TRP	ENGINEERED MUTATION	UNP Q97VT7

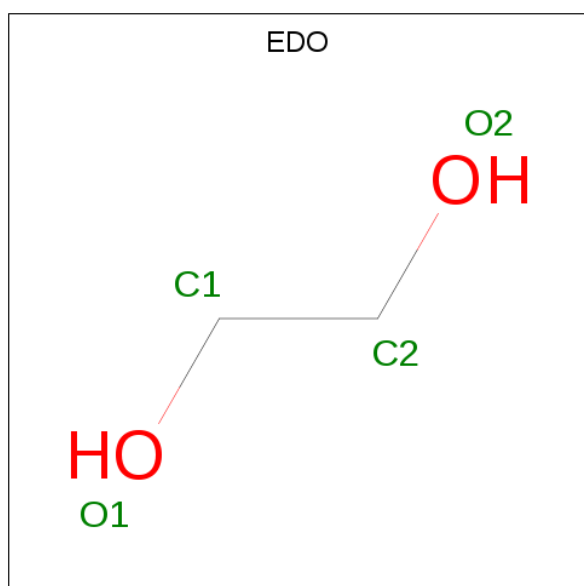
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

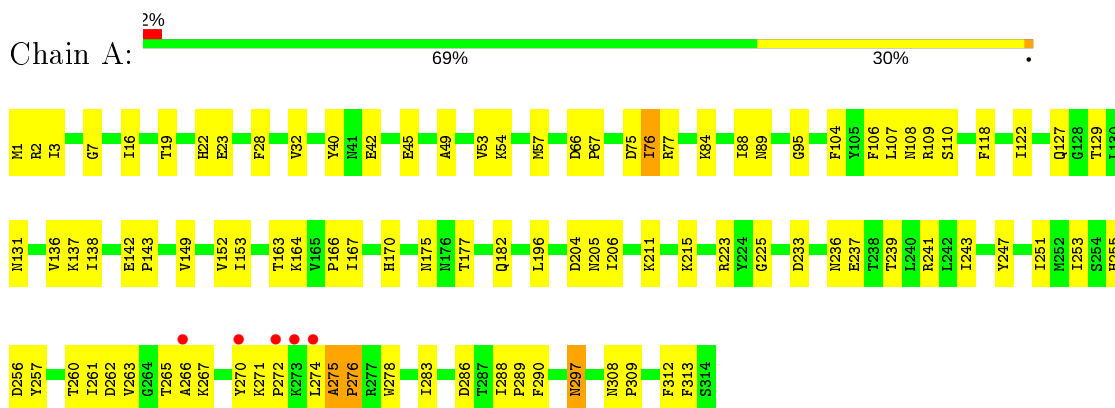
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	101	Total O 101 101	0	0
7	B	90	Total O 90 90	0	0
7	C	86	Total O 86 86	0	0
7	D	88	Total O 88 88	0	0

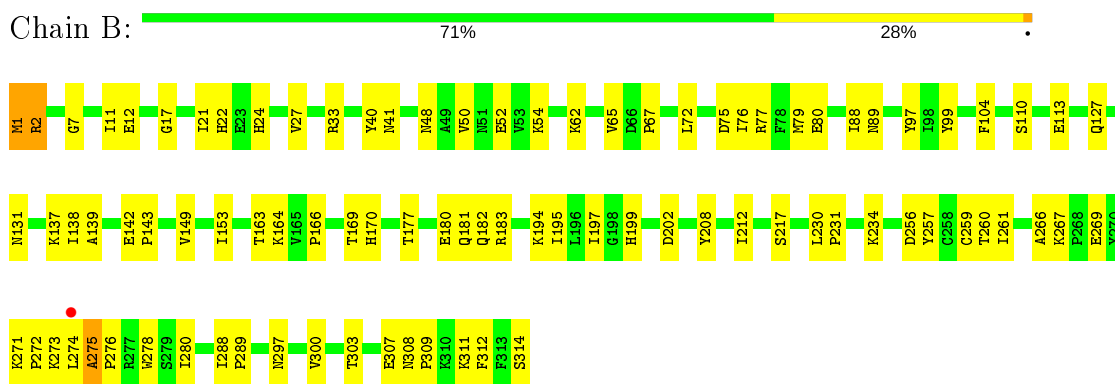
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

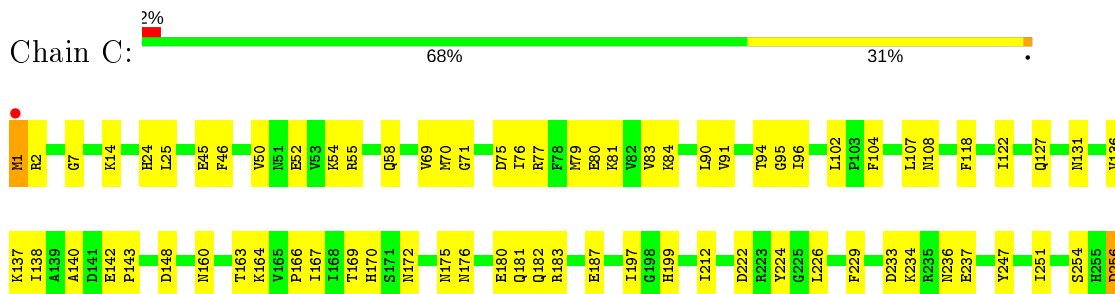
- Molecule 1: Aryldialkylphosphatase



- Molecule 1: Aryldialkylphosphatase



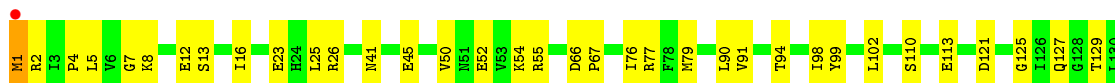
- Molecule 1: Aryldialkylphosphatase







- Molecule 1: Aryldialkylphosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.20Å 103.50Å 151.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.41 – 2.60 45.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.41-2.60) 99.7 (45.41-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.168 , 0.237 0.170 , 0.240	Depositor DCC
$R_{free}$ test set	2140 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CO, EDO, FE2, PEG, KCX

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	0.88	2/2554 (0.1%)	0.38	0/3448
1	B	0.85	2/2542 (0.1%)	0.38	0/3432
1	C	0.86	1/2542 (0.0%)	0.38	0/3432
1	D	0.85	0/2553	0.38	0/3446
All	All	0.86	5/10191 (0.0%)	0.38	0/13758

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	ILE	N-CA	6.33	1.59	1.46
1	B	256	ASP	CB-CG	5.94	1.64	1.51
1	C	256	ASP	CB-CG	5.93	1.64	1.51
1	A	256	ASP	CB-CG	5.29	1.62	1.51
1	B	22	HIS	CB-CG	5.28	1.59	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2517	0	2548	87	0
1	B	2506	0	2540	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2506	0	2540	86	0
1	D	2514	0	2553	110	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	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	12	0	18	2	0
4	D	8	0	12	1	0
5	A	12	0	16	0	0
5	B	24	0	32	3	0
5	C	12	0	16	3	0
5	D	12	0	16	4	0
6	A	7	0	10	0	0
7	A	101	0	0	15	0
7	B	90	0	0	11	0
7	C	86	0	0	7	0
7	D	88	0	0	9	0
All	All	10511	0	10313	361	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 (361) 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:D:271:LYS:CG	1:D:272:PRO:HD3	1.75	1.17
1:D:271:LYS:HG3	1:D:272:PRO:HD3	1.25	1.14
1:D:268:PRO:HA	1:D:271:LYS:HE3	1.38	1.06
1:D:26[B]:ARG:HH11	1:D:26[B]:ARG:HG2	1.14	1.04
1:D:26[B]:ARG:CG	1:D:26[B]:ARG:HH11	1.74	1.00
1:D:271:LYS:HG3	1:D:272:PRO:CD	1.98	0.94
1:B:275:ALA:H	1:B:276:PRO:CD	1.83	0.91
1:B:275:ALA:H	1:B:276:PRO:HD3	1.36	0.90
1:B:1:MET:HE3	7:B:546:HOH:O	1.70	0.90
1:D:297:ASN:HD22	1:D:299:GLU:H	1.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[B]:PHE:CE1	7:C:529:HOH:O	2.25	0.89
1:D:136:VAL:CG1	1:D:167:ILE:HG12	2.04	0.87
1:B:260:THR:OG1	7:B:590:HOH:O	1.92	0.87
1:A:106:PHE:HA	1:A:109:ARG:HG3	1.59	0.85
1:D:275:ALA:H	1:D:276:PRO:CD	1.90	0.84
1:C:84:LYS:HE2	1:C:84:LYS:HA	1.58	0.83
1:A:76:ILE:HG13	1:A:127:GLN:HE21	1.44	0.83
1:D:297:ASN:ND2	1:D:299:GLU:H	1.76	0.83
1:D:271:LYS:HG2	1:D:272:PRO:HD3	1.58	0.82
1:B:1:MET:SD	1:B:1:MET:N	2.56	0.79
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.64	0.79
1:D:4:PRO:HA	5:D:404:GOL:O3	1.84	0.77
1:D:271:LYS:CG	1:D:272:PRO:CD	2.59	0.76
1:C:163:THR:O	1:C:164:LYS:HB2	1.84	0.76
1:D:273:LYS:HG2	1:D:274:LEU:CD1	2.15	0.76
1:D:273:LYS:HG2	1:D:274:LEU:HD13	1.68	0.76
1:D:26[B]:ARG:NH1	1:D:26[B]:ARG:HG2	1.89	0.75
1:D:275:ALA:H	1:D:276:PRO:HD3	1.53	0.73
1:D:79:MET:HE3	7:D:569:HOH:O	1.88	0.73
1:C:267:LYS:HB3	1:C:269:GLU:OE2	1.89	0.73
1:A:110:SER:HB2	7:A:566:HOH:O	1.89	0.73
1:B:164:LYS:HE3	7:B:574:HOH:O	1.89	0.72
1:A:275:ALA:N	1:A:276:PRO:CD	2.53	0.72
1:B:50:VAL:O	1:B:54:LYS:HG2	1.88	0.72
1:C:142:GLU:HB2	1:C:143:PRO:HD3	1.70	0.72
1:A:104[B]:PHE:HD1	1:C:263:VAL:HG22	1.56	0.70
1:B:275:ALA:N	1:B:276:PRO:CD	2.50	0.70
1:A:2:ARG:HG3	7:A:557:HOH:O	1.90	0.69
1:D:76:ILE:HD12	1:D:77:ARG:N	2.07	0.68
1:B:97:TYR:CE1	1:B:99:TYR:HE1	2.11	0.68
1:A:275:ALA:H	1:A:276:PRO:CD	2.07	0.68
1:B:48:ASN:HD22	1:B:260:THR:CG2	2.07	0.68
1:A:297:ASN:HD22	1:A:297:ASN:H	1.39	0.68
1:A:45:GLU:HG2	1:A:260:THR:HG21	1.76	0.67
1:B:72:LEU:HG	7:B:587:HOH:O	1.95	0.67
1:A:2:ARG:HD3	7:A:590:HOH:O	1.94	0.66
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.31	0.66
1:C:197:ILE:HD12	1:C:212:ILE:CG2	2.26	0.66
1:D:275:ALA:N	1:D:276:PRO:CD	2.55	0.66
1:D:76:ILE:HD12	1:D:77:ARG:H	1.61	0.66
1:A:263:VAL:HG12	1:A:265:THR:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HD12	1:A:77:ARG:H	1.61	0.65
1:C:76:ILE:HD12	1:C:77:ARG:H	1.62	0.65
1:D:228:LEU:HA	1:D:274:LEU:HD23	1.78	0.65
1:C:197:ILE:HD12	1:C:212:ILE:HG23	1.80	0.64
1:A:149:VAL:O	1:A:153:ILE:HG13	1.98	0.64
1:A:275:ALA:N	1:A:276:PRO:HD2	2.13	0.64
1:A:257:TYR:HA	1:A:278:TRP:CZ2	2.33	0.64
1:B:76:ILE:HD12	1:B:77:ARG:N	2.13	0.63
5:B:406:GOL:H2	7:B:539:HOH:O	1.99	0.63
1:A:211:LYS:NZ	7:A:586:HOH:O	2.31	0.63
1:C:136:VAL:HG13	1:C:167:ILE:HG12	1.81	0.63
1:C:84:LYS:CA	1:C:84:LYS:HE2	2.29	0.63
1:D:26[B]:ARG:CB	1:D:26[B]:ARG:HH11	2.11	0.63
1:C:76:ILE:HD12	1:C:77:ARG:N	2.14	0.62
1:D:301:ILE:N	1:D:301:ILE:HD12	2.14	0.62
1:A:76:ILE:HD13	1:A:129:THR:HG21	1.80	0.62
1:C:81:LYS:CE	7:C:509:HOH:O	2.46	0.62
1:D:267:LYS:O	1:D:269:GLU:N	2.32	0.62
1:C:81:LYS:HE3	7:C:509:HOH:O	2.00	0.62
1:B:307:GLU:O	1:B:311:LYS:HG3	1.98	0.62
1:C:182:GLN:HB2	1:C:197:ILE:HD11	1.82	0.62
1:D:297:ASN:HD22	1:D:299:GLU:N	1.95	0.61
1:B:261:ILE:HG23	1:B:266:ALA:HB3	1.81	0.61
1:D:160:ASN:ND2	1:D:165:VAL:O	2.31	0.61
1:A:7:GLY:H	1:A:131:ASN:ND2	1.98	0.61
1:B:139:ALA:CB	1:B:170:HIS:HB3	2.31	0.61
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.36	0.61
1:C:76:ILE:HG13	1:C:127:GLN:HE21	1.66	0.61
1:B:7:GLY:H	1:B:131:ASN:ND2	1.99	0.60
1:A:53:VAL:O	1:A:57:MET:HG3	2.01	0.60
1:A:54:LYS:HD2	7:A:516:HOH:O	2.02	0.60
1:A:3:ILE:HD11	1:A:313:PHE:O	2.02	0.60
1:A:76:ILE:HG13	1:A:127:GLN:NE2	2.16	0.60
1:D:263:VAL:HG12	1:D:265:THR:H	1.67	0.60
1:A:104[B]:PHE:HE2	1:C:71:GLY:O	1.83	0.60
1:B:76:ILE:HD12	1:B:77:ARG:H	1.67	0.60
1:A:76:ILE:HD12	1:A:77:ARG:N	2.17	0.59
1:B:212:ILE:HD12	1:B:212:ILE:N	2.17	0.59
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.36	0.59
1:B:97:TYR:CE1	1:B:99:TYR:CE1	2.90	0.59
1:D:218:PHE:HZ	1:D:311:LYS:HE3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HD12	7:A:567:HOH:O	2.02	0.59
1:D:180:GLU:HA	1:D:180:GLU:OE2	2.04	0.58
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.39	0.58
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.37	0.58
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.86	0.58
1:D:218:PHE:CZ	1:D:311:LYS:HE3	2.39	0.58
1:A:308:ASN:HB2	1:A:309:PRO:HD3	1.86	0.57
1:D:136:VAL:HG13	1:D:167:ILE:HG12	1.84	0.57
1:C:257:TYR:HA	1:C:278:TRP:CZ2	2.38	0.57
1:D:274:LEU:HB2	7:D:533:HOH:O	2.05	0.57
1:A:3:ILE:CD1	1:A:313:PHE:HB3	2.35	0.57
1:B:163:THR:O	1:B:164:LYS:HB2	2.05	0.57
1:B:261:ILE:CG2	1:B:266:ALA:CB	2.83	0.57
1:C:234:LYS:HG2	7:C:572:HOH:O	2.05	0.56
1:C:288:ILE:HB	1:C:289:PRO:HD3	1.86	0.56
1:C:138:ILE:C	1:C:138:ILE:HD12	2.24	0.56
1:D:1:MET:SD	1:D:1:MET:N	2.78	0.56
1:A:28:PHE:HA	1:A:262:ASP:OD1	2.05	0.56
1:B:1:MET:CE	7:B:546:HOH:O	2.39	0.56
1:C:224:TYR:HE2	1:C:236:ASN:OD1	1.88	0.55
1:B:274:LEU:O	1:B:275:ALA:HB2	2.06	0.55
1:D:163:THR:O	1:D:164:LYS:HB2	2.05	0.55
1:D:2:ARG:HA	7:D:545:HOH:O	2.07	0.55
1:B:41:ASN:HA	7:B:581:HOH:O	2.06	0.55
1:C:271:LYS:HE2	7:C:580:HOH:O	2.07	0.55
1:D:26[B]:ARG:HB3	1:D:26[B]:ARG:NH1	2.22	0.55
1:C:46:PHE:O	1:C:50:VAL:HG23	2.07	0.55
1:C:140:ALA:HB3	1:C:181:GLN:HE21	1.72	0.55
1:D:308:ASN:HB2	1:D:309:PRO:HD3	1.89	0.55
1:C:90:LEU:HD13	1:C:91:VAL:N	2.22	0.55
1:B:208:TYR:O	1:B:212:ILE:HD13	2.06	0.54
1:C:45:GLU:HG2	1:C:260:THR:HG21	1.88	0.54
1:C:1:MET:N	1:C:1:MET:SD	2.71	0.54
1:D:137:KCX:HE3	1:D:170:HIS:HB2	1.88	0.54
1:B:27:VAL:HG13	1:B:261:ILE:HG13	1.89	0.54
1:D:274:LEU:O	1:D:275:ALA:HB2	2.06	0.54
1:D:170:HIS:ND1	1:D:199:HIS:CD2	2.76	0.54
1:A:271:LYS:HB3	1:A:272:PRO:HD3	1.90	0.54
1:B:259:CYS:O	1:B:260:THR:HG23	2.08	0.54
1:D:175:ASN:O	1:D:176:ASN:HB3	2.08	0.54
1:B:7:GLY:H	1:B:131:ASN:HD21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:OD1	1:A:177:THR:HG23	2.09	0.53
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.44	0.53
1:B:288:ILE:HB	1:B:289:PRO:HD3	1.90	0.53
1:C:258:CYS:SG	5:C:404:GOL:H12	2.49	0.53
1:C:175:ASN:O	1:C:176:ASN:HB3	2.09	0.53
1:A:76:ILE:H	1:A:127:GLN:NE2	2.07	0.53
1:B:230:LEU:HD12	1:B:231:PRO:HD2	1.91	0.53
1:C:263:VAL:HG12	1:C:265:THR:H	1.74	0.53
1:B:76:ILE:HG13	1:B:127:GLN:NE2	2.24	0.52
1:B:72:LEU:N	7:B:587:HOH:O	2.41	0.52
1:C:233:ASP:O	1:C:237:GLU:HG3	2.09	0.52
1:A:267:LYS:HB2	1:A:270:TYR:CD2	2.44	0.52
1:B:52:GLU:OE2	1:B:280:ILE:HG22	2.09	0.52
1:A:274:LEU:N	7:A:536:HOH:O	2.32	0.52
1:B:33:ARG:HG3	1:B:40:TYR:CD1	2.45	0.52
1:C:261:ILE:HG23	1:C:266:ALA:CB	2.40	0.52
1:C:261:ILE:HD11	5:C:404:GOL:H31	1.91	0.52
1:D:142:GLU:HB2	1:D:143:PRO:HD3	1.90	0.52
1:D:195:ILE:HG22	1:D:197:ILE:HD12	1.91	0.52
1:B:149:VAL:O	1:B:153:ILE:HG13	2.10	0.52
1:B:76:ILE:HG13	1:B:127:GLN:HE21	1.75	0.52
1:D:241:ARG:HD2	7:D:555:HOH:O	2.09	0.52
1:D:94:THR:O	1:D:136:VAL:HA	2.09	0.52
1:B:24:HIS:CE1	1:B:67:PRO:HG2	2.45	0.52
1:C:261:ILE:CD1	5:C:404:GOL:H31	2.40	0.52
1:C:76:ILE:HG13	1:C:127:GLN:NE2	2.25	0.52
1:C:24:HIS:CE1	1:C:137:KCX:OQ2	2.62	0.52
1:A:241:ARG:NH1	7:A:567:HOH:O	2.43	0.51
1:A:274:LEU:CA	7:A:536:HOH:O	2.58	0.51
1:B:75:ASP:O	1:B:79:MET:HG3	2.11	0.51
1:B:308:ASN:HB2	1:B:309:PRO:HD3	1.93	0.51
1:C:261:ILE:CG2	1:C:266:ALA:CB	2.88	0.51
1:A:76:ILE:H	1:A:127:GLN:HE22	1.56	0.51
1:A:267:LYS:HB2	1:A:270:TYR:HD2	1.76	0.51
1:D:2:ARG:HB2	1:D:12:GLU:HA	1.92	0.51
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.46	0.51
1:B:88:ILE:HG13	1:B:89:ASN:N	2.24	0.51
1:D:273:LYS:HG2	1:D:274:LEU:HD12	1.89	0.51
1:D:291:LEU:O	1:D:296:VAL:HB	2.11	0.51
1:C:136:VAL:CG1	1:C:167:ILE:HG12	2.41	0.51
1:C:183:ARG:O	1:C:187:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[B]:PHE:CD1	1:C:263:VAL:HG22	2.42	0.51
1:A:288:ILE:HB	1:A:289:PRO:HD3	1.91	0.51
1:B:76:ILE:O	1:B:80:GLU:N	2.41	0.51
1:D:247:TYR:O	1:D:251:ILE:HG13	2.10	0.51
1:D:16:ILE:HD12	1:D:309:PRO:HB2	1.93	0.50
1:C:104:PHE:HA	1:C:107:LEU:HD23	1.92	0.50
1:D:204:ASP:O	1:D:206:ILE:N	2.45	0.50
1:A:182:GLN:NE2	1:A:215:LYS:HB3	2.26	0.50
1:A:236:ASN:HB3	1:A:290:PHE:CE2	2.47	0.50
1:B:297:ASN:OD1	1:B:300:VAL:HG23	2.11	0.50
1:A:32:VAL:CG2	1:A:40:TYR:OH	2.60	0.50
1:A:88:ILE:HG13	1:A:89:ASN:N	2.27	0.50
1:C:261:ILE:HG23	1:C:266:ALA:HB3	1.94	0.50
1:D:5:LEU:O	5:D:404:GOL:H2	2.12	0.50
1:B:267:LYS:CD	7:D:551:HOH:O	2.58	0.50
1:D:206:ILE:HD12	1:D:241:ARG:HG2	1.93	0.50
1:B:180:GLU:OE1	1:B:183:ARG:NH1	2.41	0.49
1:C:271:LYS:N	1:C:272:PRO:CD	2.74	0.49
1:D:275:ALA:N	1:D:276:PRO:HD2	2.26	0.49
1:B:230:LEU:HD11	1:B:234:LYS:HD3	1.94	0.49
1:D:236:ASN:HB3	1:D:290:PHE:CE2	2.47	0.49
1:D:8:LYS:O	5:D:404:GOL:H31	2.12	0.49
1:B:1:MET:HE1	1:B:12:GLU:HG3	1.94	0.49
1:A:7:GLY:H	1:A:131:ASN:HD21	1.57	0.49
1:B:170:HIS:ND1	1:B:199:HIS:CD2	2.80	0.49
1:D:169:THR:OG1	1:D:197:ILE:HA	2.12	0.49
1:D:267:LYS:C	1:D:269:GLU:H	2.15	0.49
1:A:107:LEU:O	1:A:108:ASN:HB2	2.13	0.48
1:B:1:MET:CE	1:B:12:GLU:HG3	2.44	0.48
1:C:172:ASN:HB3	1:C:175:ASN:OD1	2.13	0.48
1:A:1:MET:HE2	7:A:596:HOH:O	2.13	0.48
1:B:1:MET:O	1:B:2:ARG:HB2	2.11	0.48
1:A:104[B]:PHE:HD1	1:C:263:VAL:CG2	2.25	0.48
1:B:110:SER:HA	7:B:550:HOH:O	2.12	0.48
1:D:76:ILE:HG13	1:D:127:GLN:HE21	1.77	0.48
1:C:170:HIS:ND1	1:C:199:HIS:CD2	2.80	0.48
1:D:301:ILE:CD1	1:D:301:ILE:N	2.77	0.48
1:D:16:ILE:CD1	1:D:309:PRO:HB2	2.43	0.48
1:B:76:ILE:O	1:B:80:GLU:HB2	2.13	0.48
1:D:301:ILE:H	1:D:301:ILE:CD1	2.27	0.48
1:D:4:PRO:CA	5:D:404:GOL:O3	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ILE:H	1:D:301:ILE:HD12	1.79	0.48
1:A:118:PHE:O	1:A:122:ILE:HG13	2.13	0.48
1:A:138:ILE:HD12	1:A:138:ILE:C	2.34	0.48
1:A:42:GLU:HG2	7:A:554:HOH:O	2.14	0.48
1:B:202:ASP:HB3	5:B:404:GOL:H11	1.96	0.48
1:B:195:ILE:HG22	1:B:197:ILE:HD12	1.95	0.47
1:C:264:GLY:O	1:C:267:LYS:HG3	2.13	0.47
1:B:261:ILE:HG23	1:B:266:ALA:CB	2.44	0.47
1:C:172:ASN:ND2	4:C:403:EDO:H12	2.30	0.47
1:B:234:LYS:HE3	7:B:549:HOH:O	2.15	0.47
1:C:25:LEU:O	1:C:259:CYS:HB2	2.14	0.47
1:A:136:VAL:HG13	1:A:167:ILE:HG12	1.96	0.47
1:A:239:THR:O	1:A:243:ILE:HG13	2.15	0.47
1:A:84:LYS:NZ	7:A:585:HOH:O	2.47	0.47
1:D:271:LYS:HG3	1:D:272:PRO:N	2.28	0.47
1:D:90:LEU:C	1:D:90:LEU:HD13	2.35	0.47
1:A:137:KCX:HE3	1:A:170:HIS:HB2	1.95	0.47
1:A:261:ILE:HG23	1:A:266:ALA:CB	2.44	0.47
1:D:13:SER:O	1:D:310:LYS:HG2	2.15	0.47
1:D:288:ILE:HB	1:D:289:PRO:HD3	1.96	0.47
1:A:275:ALA:H	1:A:276:PRO:HD3	1.76	0.47
1:B:2:ARG:HB3	1:B:11:ILE:O	2.14	0.47
1:B:267:LYS:HD3	7:D:551:HOH:O	2.14	0.47
1:A:16:ILE:HG22	1:A:19:THR:OG1	2.15	0.47
1:A:253:ILE:CG2	1:A:283:ILE:HD11	2.45	0.47
1:C:118:PHE:O	1:C:122:ILE:HG13	2.14	0.47
1:C:226:LEU:HD13	1:C:229:PHE:HE2	1.80	0.47
1:C:224:TYR:CE2	1:C:236:ASN:OD1	2.66	0.47
1:A:108:ASN:ND2	1:C:265:THR:OG1	2.48	0.47
1:C:52:GLU:OE2	1:C:280:ILE:HG22	2.15	0.47
1:D:76:ILE:HD13	1:D:129:THR:HG21	1.96	0.47
1:D:183:ARG:O	1:D:187:GLU:HG3	2.15	0.47
1:B:104:PHE:HE1	1:D:99:TYR:CE2	2.33	0.47
1:D:138:ILE:HD12	1:D:138:ILE:C	2.35	0.46
1:C:175:ASN:O	1:C:176:ASN:CB	2.63	0.46
1:D:23:GLU:O	1:D:66:ASP:HA	2.15	0.46
1:A:163:THR:O	1:A:164:LYS:HB2	2.16	0.46
1:A:22:HIS:CD2	1:A:67:PRO:HG2	2.50	0.46
1:B:177:THR:O	1:B:181:GLN:HG3	2.16	0.46
1:A:247:TYR:O	1:A:251:ILE:HG13	2.16	0.45
1:C:52:GLU:CD	1:C:55:ARG:HH22	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:GLU:OE1	1:D:55:ARG:NH2	2.48	0.45
1:D:7:GLY:H	1:D:131:ASN:ND2	2.14	0.45
1:D:161:LYS:NZ	1:D:161:LYS:HB3	2.31	0.45
1:B:104:PHE:CE1	1:D:99:TYR:CE2	3.04	0.45
1:B:169:THR:OG1	1:B:197:ILE:HA	2.16	0.45
1:D:218:PHE:HZ	1:D:311:LYS:CE	2.29	0.45
1:B:33:ARG:HA	1:B:40:TYR:CE1	2.51	0.45
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.16	0.45
1:D:26[B]:ARG:CB	1:D:26[B]:ARG:NH1	2.77	0.45
1:D:76:ILE:HG13	1:D:127:GLN:NE2	2.32	0.45
1:D:26[B]:ARG:HB3	1:D:26[B]:ARG:HH11	1.79	0.45
5:B:406:GOL:C2	7:B:539:HOH:O	2.63	0.45
1:B:182:GLN:NE2	1:B:217:SER:HB2	2.32	0.45
1:D:226:LEU:HD21	1:D:278:TRP:CZ2	2.52	0.45
1:A:131:ASN:HB3	7:A:594:HOH:O	2.17	0.45
1:B:142:GLU:N	1:B:143:PRO:CD	2.80	0.45
1:C:222:ASP:O	1:C:256:ASP:HB2	2.16	0.45
1:C:75:ASP:HA	1:C:127:GLN:HE22	1.82	0.44
1:C:277:ARG:HH12	1:C:286:ASP:HB2	1.82	0.44
1:D:66:ASP:OD1	1:D:66:ASP:C	2.55	0.44
1:A:255:HIS:NE2	1:A:283:ILE:HB	2.32	0.44
1:A:95:GLY:HA2	1:A:118:PHE:CE1	2.53	0.44
1:C:180:GLU:OE1	1:C:183:ARG:NH1	2.44	0.44
1:C:14:LYS:HD3	1:C:310:LYS:HD3	1.99	0.44
1:B:271:LYS:HB3	1:B:272:PRO:CD	2.42	0.44
1:B:303:THR:HA	1:B:307:GLU:HB2	1.99	0.44
1:A:104[B]:PHE:CE2	1:C:71:GLY:O	2.67	0.44
1:D:121:ASP:HA	1:D:125:GLY:O	2.17	0.44
1:C:296:VAL:HG12	1:C:301:ILE:CD1	2.47	0.44
1:C:90:LEU:HD13	1:C:90:LEU:C	2.38	0.44
1:D:273:LYS:HB2	1:D:273:LYS:NZ	2.33	0.44
1:B:21:ILE:HD12	1:B:65:VAL:HG21	2.00	0.44
1:D:261:ILE:HG23	1:D:266:ALA:HB3	1.99	0.44
1:A:251:ILE:O	1:A:308:ASN:ND2	2.46	0.44
1:C:102:LEU:HG	1:C:148:ASP:HB3	2.00	0.44
1:A:75:ASP:HA	1:A:127:GLN:HE22	1.83	0.43
1:D:5:LEU:HD23	1:D:91:VAL:HG22	2.00	0.43
1:C:138:ILE:HD11	1:C:169:THR:HB	2.00	0.43
1:C:94:THR:O	1:C:136:VAL:HA	2.18	0.43
1:A:233:ASP:N	1:A:233:ASP:OD1	2.51	0.43
1:A:271:LYS:N	1:A:272:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:C	7:A:536:HOH:O	2.55	0.43
1:B:194:LYS:NZ	1:B:314:SER:O	2.43	0.43
1:D:267:LYS:C	1:D:269:GLU:N	2.72	0.43
1:A:142:GLU:N	1:A:143:PRO:CD	2.82	0.43
1:C:277:ARG:NH2	7:C:532:HOH:O	2.48	0.43
1:D:197:ILE:N	1:D:197:ILE:HD12	2.33	0.43
1:A:76:ILE:HD13	1:A:129:THR:CG2	2.48	0.43
1:C:197:ILE:HD12	1:C:212:ILE:HG21	2.00	0.43
4:C:403:EDO:H11	7:C:515:HOH:O	2.18	0.43
1:B:17:GLY:HA3	1:B:62:LYS:HD3	2.00	0.43
1:A:170:HIS:HE1	1:A:223:ARG:HH22	1.67	0.43
1:A:225:GLY:N	7:A:592:HOH:O	2.29	0.43
1:B:163:THR:O	1:B:164:LYS:CB	2.67	0.42
1:A:297:ASN:N	1:A:297:ASN:HD22	2.13	0.42
1:D:50:VAL:O	1:D:54:LYS:HG2	2.20	0.42
1:C:226:LEU:HD13	1:C:229:PHE:CE2	2.54	0.42
1:D:26[B]:ARG:HD2	1:D:45:GLU:CD	2.39	0.42
1:B:110:SER:OG	1:B:113:GLU:HG3	2.20	0.42
1:B:182:GLN:HE21	1:B:217:SER:CB	2.33	0.42
1:C:7:GLY:H	1:C:131:ASN:ND2	2.18	0.42
1:D:310:LYS:HB3	1:D:310:LYS:HE2	1.79	0.42
4:D:403:EDO:H12	7:D:549:HOH:O	2.18	0.42
1:A:138:ILE:HG22	1:A:152:VAL:HG12	2.00	0.42
1:A:233:ASP:O	1:A:237:GLU:OE1	2.37	0.42
1:B:208:TYR:O	1:B:212:ILE:CD1	2.68	0.42
1:C:160:ASN:O	1:C:164:LYS:N	2.47	0.42
1:D:98:ILE:HD13	1:D:102:LEU:HD23	2.02	0.42
1:D:79:MET:CE	7:D:569:HOH:O	2.59	0.42
1:C:70:MET:CE	1:C:96:ILE:HG23	2.50	0.42
1:C:79:MET:O	1:C:83:VAL:HG23	2.19	0.41
1:D:67:PRO:HB2	1:D:137:KCX:HG2	2.01	0.41
1:D:110:SER:OG	1:D:113:GLU:HG3	2.20	0.41
1:B:267:LYS:O	1:B:269:GLU:N	2.54	0.41
1:C:107:LEU:O	1:C:108:ASN:HB2	2.21	0.41
1:D:147:LYS:HE2	7:D:578:HOH:O	2.18	0.41
1:D:137:KCX:OQ2	1:D:170:HIS:HB2	2.20	0.41
1:D:25:LEU:O	1:D:259:CYS:HB2	2.20	0.41
1:B:212:ILE:CD1	1:B:212:ILE:N	2.82	0.41
1:A:49:ALA:O	1:A:53:VAL:HG23	2.20	0.41
1:B:139:ALA:HB2	1:B:170:HIS:HB3	2.02	0.41
1:C:261:ILE:HG12	1:C:263:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:HD12	1:D:231:PRO:HD2	2.01	0.41
1:A:23:GLU:O	1:A:66:ASP:HA	2.20	0.41
1:D:255:HIS:NE2	1:D:283:ILE:HG23	2.35	0.41
1:D:41:ASN:O	1:D:45:GLU:HG3	2.20	0.41
1:A:204:ASP:O	1:A:206:ILE:N	2.53	0.41
1:C:308:ASN:HB2	1:C:309:PRO:HD3	2.03	0.41
1:A:137:KCX:OQ2	1:A:170:HIS:HB2	2.21	0.41
1:C:69:VAL:HG11	1:C:137:KCX:HB2	2.03	0.41
1:D:175:ASN:O	1:D:176:ASN:CB	2.69	0.41
1:D:271:LYS:N	1:D:272:PRO:CD	2.84	0.41
1:C:183:ARG:HD2	1:C:187:GLU:OE1	2.21	0.41
1:D:2:ARG:HG3	1:D:12:GLU:HG2	2.02	0.40
1:A:253:ILE:HG21	1:A:283:ILE:HD11	2.03	0.40
1:A:286:ASP:C	1:A:286:ASP:OD1	2.59	0.40
1:B:137:KCX:HE3	1:B:170:HIS:HB2	2.03	0.40
1:B:138:ILE:HD11	1:B:169:THR:HG22	2.03	0.40
1:B:142:GLU:HB2	1:B:143:PRO:HD3	2.03	0.40
1:C:80:GLU:O	1:C:84:LYS:HG2	2.21	0.40
1:C:277:ARG:NH1	1:C:286:ASP:HB2	2.37	0.40
1:C:247:TYR:O	1:C:251:ILE:HG13	2.21	0.40
1:C:54:LYS:O	1:C:58:GLN:HG3	2.21	0.40
1:D:136:VAL:HG12	1:D:167:ILE:HG12	1.96	0.40
1:D:271:LYS:N	1:D:272:PRO:HD2	2.36	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	312/314 (99%)	296 (95%)	13 (4%)	3 (1%)	15 32
1	B	311/314 (99%)	294 (94%)	14 (4%)	3 (1%)	15 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	311/314 (99%)	290 (93%)	21 (7%)	0	100	100
1	D	312/314 (99%)	290 (93%)	18 (6%)	4 (1%)	12	24
All	All	1246/1256 (99%)	1170 (94%)	66 (5%)	10 (1%)	19	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	B	275	ALA
1	D	205	ASN
1	D	275	ALA
1	B	2	ARG
1	B	273	LYS
1	D	268	PRO
1	D	276	PRO
1	A	275	ALA
1	A	276	PRO

### 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	273/272 (100%)	271 (99%)	2 (1%)	84	94
1	B	272/272 (100%)	271 (100%)	1 (0%)	91	97
1	C	272/272 (100%)	268 (98%)	4 (2%)	65	83
1	D	273/272 (100%)	271 (99%)	2 (1%)	84	94
All	All	1090/1088 (100%)	1081 (99%)	9 (1%)	81	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LEU
1	A	297	ASN

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Mol	Chain	Res	Type
1	B	1	MET
1	C	1	MET
1	C	2	ARG
1	C	254	SER
1	C	277	ARG
1	D	1	MET
1	D	297	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	51	ASN
1	A	58	GLN
1	A	108	ASN
1	A	127	GLN
1	A	131	ASN
1	A	294	ASN
1	A	297	ASN
1	B	48	ASN
1	B	127	GLN
1	B	131	ASN
1	C	108	ASN
1	C	127	GLN
1	C	131	ASN
1	C	294	ASN
1	D	34	GLN
1	D	51	ASN
1	D	58	GLN
1	D	127	GLN
1	D	131	ASN
1	D	294	ASN
1	D	297	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	D	137	1,3	7,11,12	0.87	0	4,12,14	0.39	0
1	KCX	B	137	1,3	7,11,12	0.61	0	4,12,14	0.40	0
1	KCX	C	137	1,3	7,11,12	1.42	1 (14%)	4,12,14	0.40	0
1	KCX	A	137	1,3	7,11,12	0.84	0	4,12,14	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	D	137	1,3	-	3/7/10/12	-
1	KCX	B	137	1,3	-	4/7/10/12	-
1	KCX	C	137	1,3	-	0/7/10/12	-
1	KCX	A	137	1,3	-	4/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	KCX	CB-CA	2.61	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	137	KCX	N-CA-CB-CG
1	D	137	KCX	C-CA-CB-CG
1	B	137	KCX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	137	KCX	N-CA-CB-CG
1	A	137	KCX	C-CA-CB-CG
1	B	137	KCX	CG-CD-CE-NZ
1	B	137	KCX	CA-CB-CG-CD
1	A	137	KCX	CA-CB-CG-CD
1	B	137	KCX	N-CA-CB-CG
1	D	137	KCX	CA-CB-CG-CD
1	A	137	KCX	CG-CD-CE-NZ

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	137	KCX	3	0
1	B	137	KCX	1	0
1	C	137	KCX	2	0
1	A	137	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	EDO	C	407	-	3,3,3	0.51	0	2,2,2	0.33	0
5	GOL	A	404	-	5,5,5	0.30	0	5,5,5	0.31	0
5	GOL	C	404	-	5,5,5	0.64	0	5,5,5	0.20	0
4	EDO	C	403	-	3,3,3	0.46	0	2,2,2	0.34	0
5	GOL	D	405	-	5,5,5	0.23	0	5,5,5	0.27	0
5	GOL	B	406	-	5,5,5	0.42	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	404	-	5,5,5	0.54	0	5,5,5	0.30	0
5	GOL	B	405	-	5,5,5	0.22	0	5,5,5	0.32	0
5	GOL	A	405	-	5,5,5	0.40	0	5,5,5	0.29	0
5	GOL	C	405	-	5,5,5	0.14	0	5,5,5	0.29	0
4	EDO	D	403	-	3,3,3	0.64	0	2,2,2	0.34	0
5	GOL	D	404	-	5,5,5	0.15	0	5,5,5	0.32	0
4	EDO	B	403	-	3,3,3	0.97	0	2,2,2	0.27	0
4	EDO	C	406	-	3,3,3	0.52	0	2,2,2	0.35	0
4	EDO	D	406	-	3,3,3	0.35	0	2,2,2	0.38	0
6	PEG	A	406	-	6,6,6	0.85	0	5,5,5	0.26	0
5	GOL	B	407	-	5,5,5	0.42	0	5,5,5	0.25	0
4	EDO	A	403	-	3,3,3	0.61	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	407	-	-	1/1/1/1	-
5	GOL	A	404	-	-	4/4/4/4	-
5	GOL	C	404	-	-	2/4/4/4	-
4	EDO	C	403	-	-	1/1/1/1	-
5	GOL	D	405	-	-	0/4/4/4	-
5	GOL	B	406	-	-	4/4/4/4	-
5	GOL	B	404	-	-	2/4/4/4	-
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	A	405	-	-	4/4/4/4	-
5	GOL	C	405	-	-	2/4/4/4	-
4	EDO	D	403	-	-	0/1/1/1	-
5	GOL	D	404	-	-	4/4/4/4	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	406	-	-	1/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
6	PEG	A	406	-	-	3/4/4/4	-
5	GOL	B	407	-	-	2/4/4/4	-
4	EDO	A	403	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GOL	O1-C1-C2-C3
5	A	404	GOL	C1-C2-C3-O3
5	B	404	GOL	O1-C1-C2-C3
5	B	406	GOL	O1-C1-C2-C3
5	B	406	GOL	C1-C2-C3-O3
5	B	406	GOL	O2-C2-C3-O3
5	B	405	GOL	O1-C1-C2-C3
5	A	405	GOL	O1-C1-C2-O2
5	A	405	GOL	O1-C1-C2-C3
5	A	405	GOL	C1-C2-C3-O3
5	C	405	GOL	O1-C1-C2-O2
4	C	407	EDO	O1-C1-C2-O2
5	B	404	GOL	O1-C1-C2-O2
5	A	405	GOL	O2-C2-C3-O3
6	A	406	PEG	O1-C1-C2-O2
6	A	406	PEG	O2-C3-C4-O4
5	C	404	GOL	O1-C1-C2-C3
5	C	405	GOL	O1-C1-C2-C3
5	D	404	GOL	O1-C1-C2-C3
5	D	404	GOL	C1-C2-C3-O3
5	A	404	GOL	O2-C2-C3-O3
5	B	406	GOL	O1-C1-C2-O2
5	B	405	GOL	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
5	D	404	GOL	O2-C2-C3-O3
5	A	404	GOL	O1-C1-C2-O2
5	C	404	GOL	O1-C1-C2-O2
5	D	404	GOL	O1-C1-C2-O2
4	C	406	EDO	O1-C1-C2-O2
6	A	406	PEG	C4-C3-O2-C2
4	D	406	EDO	O1-C1-C2-O2
5	B	407	GOL	C1-C2-C3-O3
5	B	407	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	EDO	2	0
5	B	406	GOL	2	0
5	B	404	GOL	1	0
4	D	403	EDO	1	0
5	D	404	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	313/314 (99%)	-0.37	5 (1%) 72 68	20, 31, 53, 86	1 (0%)
1	B	313/314 (99%)	-0.48	1 (0%) 94 93	21, 32, 55, 89	1 (0%)
1	C	313/314 (99%)	-0.28	5 (1%) 72 68	21, 34, 57, 87	1 (0%)
1	D	313/314 (99%)	-0.31	9 (2%) 51 45	24, 36, 60, 98	1 (0%)
All	All	1252/1256 (99%)	-0.36	20 (1%) 72 68	20, 33, 57, 98	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	PRO	4.5
1	A	266	ALA	4.1
1	D	270	TYR	3.9
1	D	1	MET	3.9
1	A	274	LEU	3.8
1	D	268	PRO	3.8
1	C	268	PRO	3.7
1	D	271	LYS	3.0
1	A	273	LYS	3.0
1	B	274	LEU	2.8
1	D	266	ALA	2.6
1	C	266	ALA	2.5
1	C	271	LYS	2.5
1	A	272	PRO	2.4
1	D	267	LYS	2.3
1	D	274	LEU	2.3
1	C	1	MET	2.1
1	A	270	TYR	2.0
1	C	270	TYR	2.0
1	D	273	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	D	137	12/13	0.97	0.14	24,27,30,30	0
1	KCX	B	137	12/13	0.98	0.12	21,21,22,23	0
1	KCX	C	137	12/13	0.98	0.12	22,24,26,29	0
1	KCX	A	137	12/13	0.98	0.14	21,21,23,23	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	403	4/4	0.73	0.48	40,50,50,51	0
6	PEG	A	406	7/7	0.77	0.19	45,52,57,62	0
4	EDO	C	406	4/4	0.79	0.24	49,52,57,57	0
5	GOL	C	404	6/6	0.86	0.17	57,65,68,72	0
5	GOL	B	406	6/6	0.88	0.25	47,49,53,61	0
5	GOL	B	407	6/6	0.88	0.23	50,53,59,64	0
4	EDO	A	403	4/4	0.88	0.23	49,49,49,50	0
5	GOL	B	404	6/6	0.88	0.22	44,44,45,46	0
4	EDO	D	406	4/4	0.89	0.23	51,52,54,58	0
4	EDO	C	407	4/4	0.89	0.18	49,55,57,63	0
5	GOL	D	404	6/6	0.89	0.23	48,50,52,63	0
5	GOL	A	405	6/6	0.92	0.17	47,51,53,54	0
5	GOL	C	405	6/6	0.94	0.20	48,48,53,54	0
4	EDO	C	403	4/4	0.94	0.33	46,51,53,57	0
4	EDO	D	403	4/4	0.95	0.20	34,37,37,41	0
5	GOL	D	405	6/6	0.95	0.19	49,52,53,54	0
5	GOL	A	404	6/6	0.97	0.14	33,37,38,38	0
5	GOL	B	405	6/6	0.97	0.16	37,41,42,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	D	401	1/1	0.98	0.09	23,23,23,23	0
3	CO	C	402	1/1	0.99	0.09	33,33,33,33	0
3	CO	A	402	1/1	0.99	0.10	27,27,27,27	0
2	FE2	A	401	1/1	0.99	0.10	22,22,22,22	0
2	FE2	C	401	1/1	0.99	0.09	21,21,21,21	0
2	FE2	B	401	1/1	1.00	0.09	23,23,23,23	0
3	CO	D	402	1/1	1.00	0.09	28,28,28,28	0
3	CO	B	402	1/1	1.00	0.09	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.