



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:48 am GMT

PDB ID : 4OOJ
Title : Crystal structure of the N-terminal domain of the Legionella pneumophila protein SidC at 2.4Å resolution
Authors : Gazdag, E.M.; Shoebel, S.; Shkumatov, A.V.; Goody, R.S.; Itzen, A.
Deposited on : 2014-02-03
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

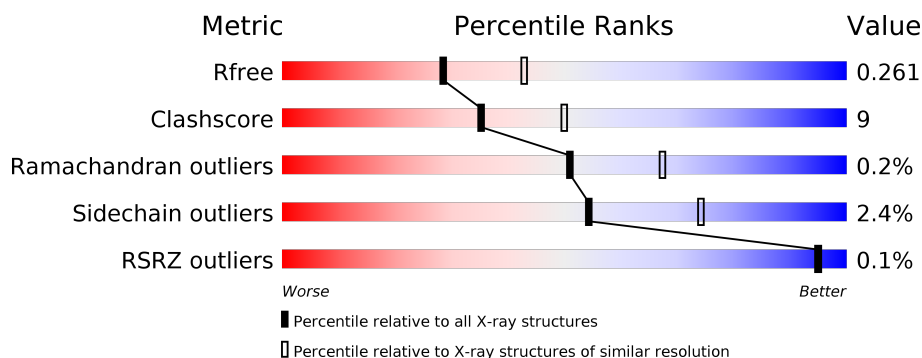
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	611	 83% 14% ..
1	B	611	 83% 15% .
1	C	611	 82% 17% .
1	D	611	 81% 18% .

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	701	-	-	-	X
3	PEG	A	702	-	-	-	X
3	PEG	A	703	-	-	-	X
3	PEG	A	704	-	-	-	X
3	PEG	A	705	-	-	X	X
3	PEG	A	706	-	-	X	X
3	PEG	B	703	-	-	X	-
3	PEG	B	704	-	-	X	-
3	PEG	C	703	-	-	-	X
3	PEG	D	702	-	-	X	X
3	PEG	D	703	-	-	-	X
3	PEG	D	706	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20006 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 SidC, interaptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	1	0
			4833	3053	823	951	6			
1	B	608	Total	C	N	O	S	0	0	0
			4856	3065	824	960	7			
1	C	611	Total	C	N	O	S	0	1	0
			4886	3086	829	963	8			
1	D	610	Total	C	N	O	S	0	1	0
			4889	3091	834	956	8			

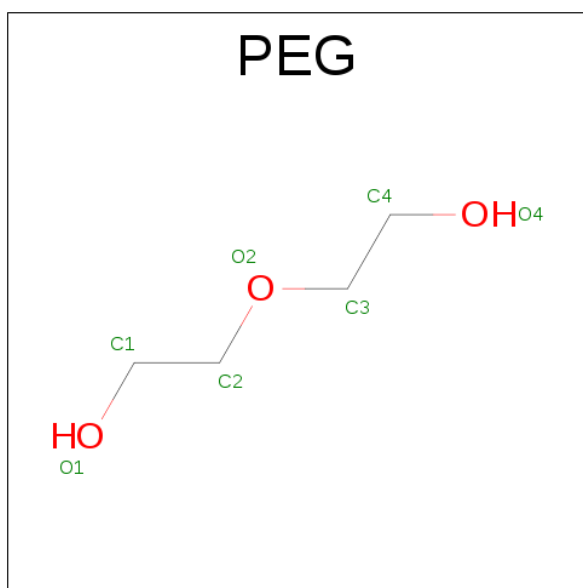
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q5ZSK6
A	0	PRO	-	EXPRESSION TAG	UNP Q5ZSK6
B	-1	GLY	-	EXPRESSION TAG	UNP Q5ZSK6
B	0	PRO	-	EXPRESSION TAG	UNP Q5ZSK6
C	-1	GLY	-	EXPRESSION TAG	UNP Q5ZSK6
C	0	PRO	-	EXPRESSION TAG	UNP Q5ZSK6
D	-1	GLY	-	EXPRESSION TAG	UNP Q5ZSK6
D	0	PRO	-	EXPRESSION TAG	UNP Q5ZSK6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

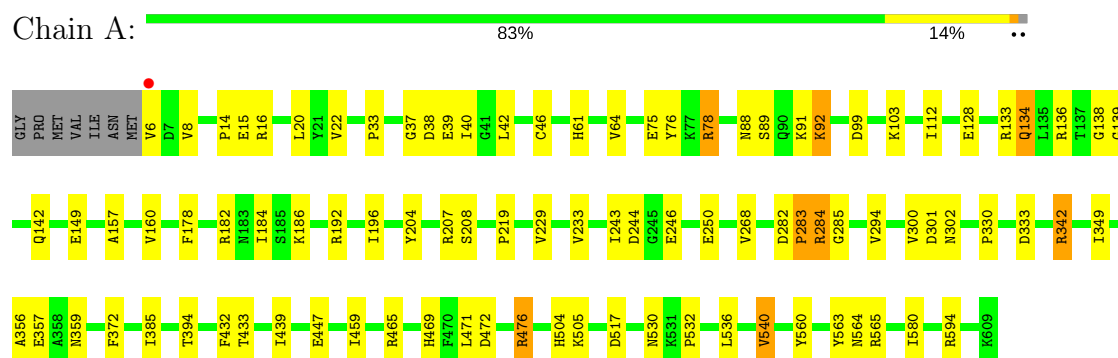
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	118	Total O 118 118	0	0
4	B	109	Total O 109 109	0	0
4	C	90	Total O 90 90	0	0
4	D	102	Total O 102 102	0	0

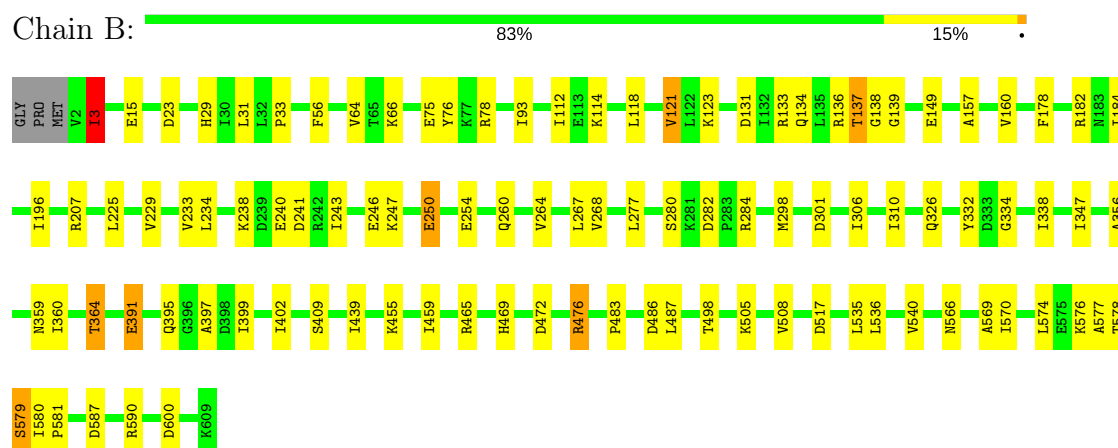
3 Residue-property plots

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.

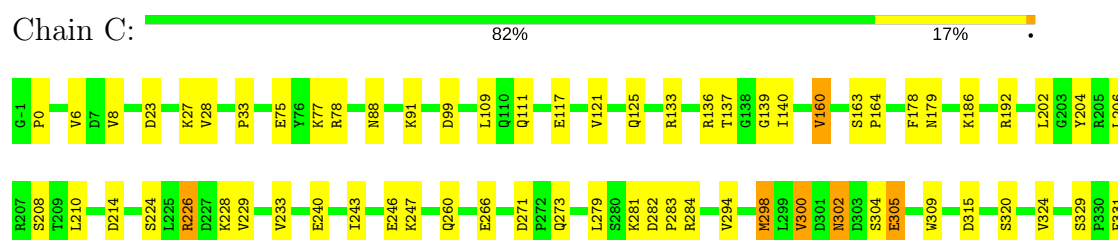
• Molecule 1: SidC, interaptin

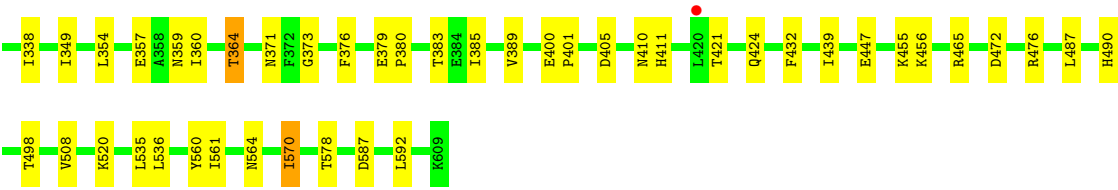


• Molecule 1: SidC, interaptin

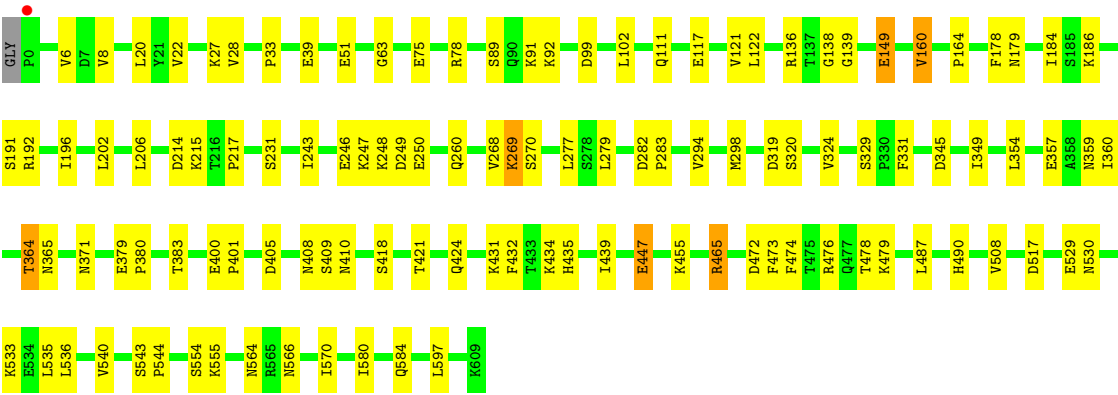
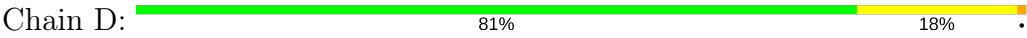


• Molecule 1: SidC, interaptin





● Molecule 1: SidC, interaptin



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	119.06Å 119.06Å 201.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.90 – 2.40 45.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.90-2.40) 99.8 (45.90-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.262 0.201 , 0.261	Depositor DCC
R_{free} test set	6240 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.488 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20006	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.53% 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, 0.333 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: MG, PEG

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	0.92	5/4933 (0.1%)	0.86	7/6681 (0.1%)
1	B	0.91	2/4955 (0.0%)	0.85	7/6713 (0.1%)
1	C	0.86	2/4989 (0.0%)	0.82	2/6757 (0.0%)
1	D	0.87	3/4992 (0.1%)	0.81	1/6755 (0.0%)
All	All	0.89	12/19869 (0.1%)	0.83	17/26906 (0.1%)

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	B	0	3
1	C	0	1
1	D	0	1
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	GLU	CB-CG	-9.07	1.34	1.52
1	C	447	GLU	CB-CG	-6.60	1.39	1.52
1	C	117	GLU	CG-CD	6.34	1.61	1.51
1	A	46	CYS	CB-SG	6.14	1.92	1.82
1	A	128	GLU	CG-CD	5.40	1.60	1.51
1	D	447	GLU	CB-CG	-5.38	1.42	1.52
1	D	149	GLU	CG-CD	5.33	1.59	1.51
1	B	391	GLU	CB-CG	5.21	1.62	1.52
1	A	78	ARG	CG-CD	5.16	1.64	1.51
1	A	134	GLN	CB-CG	-5.12	1.38	1.52
1	B	391	GLU	CG-CD	5.12	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	GLU	CG-CD	5.07	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	B	207	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	476	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	A	207	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	476	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	465	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	207	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	476	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	207	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	301	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	301	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	226	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	284	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	277	LEU	CA-CB-CG	5.29	127.46	115.30
1	C	139	GLY	N-CA-C	-5.20	100.09	113.10
1	A	447	GLU	N-CA-CB	-5.09	101.43	110.60
1	B	301	ASP	CB-CG-OD2	-5.08	113.72	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	THR	Peptide
1	B	3	ILE	Peptide
1	B	576	LYS	Peptide
1	C	137	THR	Peptide
1	D	243	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4833	0	4690	86	0
1	B	4856	0	4710	97	0
1	C	4886	0	4752	79	1
1	D	4889	0	4783	100	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	42	0	60	27	1
3	B	28	0	40	28	0
3	C	14	0	20	1	0
3	D	35	0	50	20	0
4	A	118	0	0	11	0
4	B	109	0	0	11	0
4	C	90	0	0	6	0
4	D	102	0	0	7	0
All	All	20006	0	19105	360	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (360) 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:B:137:THR:CG2	3:B:704:PEG:H12	1.62	1.29
1:D:136[B]:ARG:NH2	4:D:824:HOH:O	1.66	1.28
1:B:149:GLU:CG	3:B:703:PEG:H41	1.76	1.14
1:B:137:THR:HG21	3:B:704:PEG:H12	1.32	1.10
1:B:149:GLU:HG3	3:B:703:PEG:H41	1.11	1.08
1:B:364:THR:HG21	4:B:887:HOH:O	1.52	1.07
3:B:704:PEG:H21	4:B:898:HOH:O	1.59	1.02
1:B:149:GLU:HG3	3:B:703:PEG:C4	1.90	1.00
1:A:134:GLN:HE22	1:A:142:GLN:H	1.07	1.00
1:D:246:GLU:HA	3:D:706:PEG:O1	1.60	1.00
1:A:61:HIS:O	1:A:64:VAL:HG12	1.68	0.93
1:B:137:THR:HG22	3:B:704:PEG:H12	1.51	0.91
1:D:535:LEU:HD23	1:D:570:ILE:HD13	1.53	0.90
1:A:38:ASP:H	3:A:705:PEG:H21	1.36	0.89
1:A:92:LYS:HE3	3:A:706:PEG:C3	2.02	0.88
1:B:137:THR:CG2	3:B:704:PEG:C1	2.51	0.87
1:A:244:ASP:HB3	4:A:890:HOH:O	1.74	0.85
1:C:379:GLU:OE1	1:C:383:THR:OG1	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:NH2	4:C:890:HOH:O	2.10	0.84
1:A:89:SER:HA	3:A:706:PEG:H41	1.58	0.83
1:B:160:VAL:HG22	1:B:178:PHE:HB3	1.62	0.82
1:A:39:GLU:H	3:A:705:PEG:H32	1.46	0.81
1:C:535:LEU:HD23	1:C:570:ILE:HD13	1.62	0.81
1:D:28:VAL:H	1:D:111:GLN:NE2	1.77	0.81
1:A:136:ARG:NH2	4:A:918:HOH:O	2.13	0.80
1:D:246:GLU:CA	3:D:706:PEG:O1	2.28	0.80
1:D:247:LYS:H	3:D:706:PEG:C1	1.94	0.80
1:A:89:SER:HA	3:A:706:PEG:C4	2.11	0.80
1:A:282:ASP:OD2	1:A:283:PRO:HD2	1.82	0.80
1:A:540:VAL:HG21	1:A:580:ILE:HD12	1.61	0.79
1:B:137:THR:HG22	1:B:138:GLY:N	1.97	0.79
4:A:917:HOH:O	1:B:298:MET:HE2	1.82	0.78
1:D:149:GLU:OE2	4:D:860:HOH:O	2.01	0.78
1:A:16:ARG:O	3:A:702:PEG:H41	1.84	0.78
1:A:38:ASP:HB3	3:A:705:PEG:H31	1.66	0.77
1:A:6:VAL:HG12	1:A:8:VAL:HG12	1.65	0.77
1:B:574:LEU:O	1:B:577:ALA:HB2	1.85	0.77
1:D:379:GLU:O	1:D:383:THR:HG22	1.86	0.76
1:B:182:ARG:HE	3:B:702:PEG:H22	1.50	0.75
3:B:704:PEG:H42	4:B:899:HOH:O	1.87	0.74
1:C:133:ARG:HD3	4:C:890:HOH:O	1.88	0.74
1:A:138:GLY:O	1:B:284:ARG:NH1	2.19	0.74
1:C:75[A]:GLU:OE1	1:C:78:ARG:NH1	2.19	0.74
1:D:27:LYS:HA	1:D:111:GLN:HE22	1.52	0.73
1:A:134:GLN:HE22	1:A:142:GLN:N	1.86	0.72
1:B:326:GLN:HA	1:B:326:GLN:OE1	1.89	0.72
1:B:133:ARG:HD2	3:B:704:PEG:H32	1.71	0.72
1:D:247:LYS:N	3:D:706:PEG:O1	2.21	0.72
1:B:137:THR:CG2	1:B:138:GLY:N	2.52	0.71
1:A:134:GLN:NE2	4:A:877:HOH:O	2.18	0.71
1:D:39:GLU:OE1	1:D:434:LYS:NZ	2.21	0.71
1:D:364:THR:HG23	1:D:455:LYS:HD2	1.73	0.70
1:A:75:GLU:OE2	1:A:78:ARG:NH1	2.24	0.70
1:C:202:LEU:HD23	1:C:206:LEU:HD12	1.75	0.69
1:D:564:ASN:HD22	1:D:566:ASN:H	1.38	0.69
1:D:249:ASP:OD1	4:D:870:HOH:O	2.11	0.69
1:A:469:HIS:HD1	1:A:471:LEU:H	1.41	0.69
1:C:28:VAL:H	1:C:111:GLN:HE22	1.40	0.69
1:C:28:VAL:H	1:C:111:GLN:NE2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:ASN:ND2	1:D:566:ASN:H	1.90	0.68
1:D:28:VAL:H	1:D:111:GLN:HE22	1.42	0.68
1:A:139:GLY:N	4:A:860:HOH:O	2.27	0.67
1:D:401:PRO:O	1:D:405:ASP:N	2.22	0.67
1:B:465:ARG:HH21	3:B:705:PEG:H31	1.59	0.67
1:A:61:HIS:O	1:A:64:VAL:CG1	2.43	0.67
1:B:137:THR:HB	3:B:704:PEG:C1	2.25	0.66
1:A:37:GLY:HA2	3:A:705:PEG:H11	1.78	0.66
1:B:225:LEU:HD21	1:B:267:LEU:HD21	1.77	0.66
1:B:133:ARG:CD	3:B:704:PEG:H32	2.26	0.66
1:B:160:VAL:HG21	1:B:356:ALA:HB1	1.77	0.65
1:A:92:LYS:HE3	3:A:706:PEG:H31	1.78	0.65
1:B:391:GLU:OE2	1:B:395:GLN:NE2	2.30	0.65
1:D:365:ASN:HD21	1:D:455:LYS:NZ	1.96	0.64
1:A:15:GLU:OE2	1:A:505:LYS:HE2	1.97	0.64
1:A:178:PHE:HD2	1:A:359:ASN:HD22	1.45	0.64
1:D:379:GLU:OE1	1:D:383:THR:CG2	2.46	0.64
1:A:39:GLU:N	3:A:705:PEG:H32	2.13	0.64
1:A:39:GLU:H	3:A:705:PEG:C3	2.11	0.64
1:C:202:LEU:CD2	1:C:206:LEU:HD12	2.28	0.63
1:A:149:GLU:OE1	4:A:868:HOH:O	2.16	0.63
1:A:284:ARG:NH1	1:B:137:THR:O	2.32	0.62
1:C:320:SER:O	1:C:324:VAL:HG13	2.00	0.62
1:B:3:ILE:H	1:B:3:ILE:HD12	1.65	0.61
1:D:331:PHE:CE2	1:D:354:LEU:HD22	2.36	0.61
1:C:243:ILE:HD13	1:C:309:TRP:CD1	2.36	0.60
1:A:92:LYS:HE3	3:A:706:PEG:C4	2.31	0.60
1:B:137:THR:HG22	1:B:138:GLY:HA3	1.82	0.60
1:B:178:PHE:HD2	1:B:359:ASN:HD22	1.47	0.60
1:B:29:HIS:HD2	1:B:469:HIS:HE2	1.49	0.60
1:A:284:ARG:NH1	1:B:139:GLY:O	2.35	0.60
1:B:137:THR:HG22	1:B:138:GLY:CA	2.31	0.60
1:C:520:LYS:NZ	3:C:703:PEG:H11	2.17	0.60
1:B:540:VAL:HG21	1:B:580:ILE:HD12	1.84	0.60
1:C:202:LEU:CD2	1:C:206:LEU:CD1	2.80	0.59
1:C:439:ILE:C	1:C:439:ILE:HD12	2.22	0.59
1:A:134:GLN:NE2	1:A:142:GLN:H	1.89	0.59
1:D:247:LYS:N	3:D:706:PEG:C1	2.63	0.59
1:B:137:THR:CB	3:B:704:PEG:H12	2.29	0.59
1:C:487:LEU:HA	1:C:490:HIS:CD2	2.37	0.59
1:B:243:ILE:HG22	1:B:243:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HD21	1:B:267:LEU:CD2	2.32	0.59
1:B:137:THR:CB	3:B:704:PEG:C1	2.80	0.58
1:D:439:ILE:HD12	1:D:439:ILE:C	2.22	0.58
1:A:182:ARG:HE	3:A:703:PEG:H32	1.68	0.58
1:D:247:LYS:H	3:D:706:PEG:H11	1.65	0.58
1:D:99:ASP:OD1	3:D:702:PEG:H42	2.03	0.58
1:C:456:LYS:HA	4:C:870:HOH:O	2.03	0.58
1:D:319:ASP:OD1	1:D:320:SER:N	2.36	0.58
1:D:487:LEU:HA	1:D:490:HIS:CD2	2.39	0.58
1:A:229:VAL:O	1:A:233:VAL:HG23	2.04	0.57
1:D:268:VAL:O	1:D:270:SER:N	2.36	0.57
1:C:379:GLU:OE1	1:C:379:GLU:O	2.22	0.57
1:C:23:ASP:O	1:C:508:VAL:HG21	2.05	0.57
1:B:15:GLU:CD	1:B:505:LYS:NZ	2.57	0.57
1:A:138:GLY:O	1:B:284:ARG:NH2	2.37	0.56
1:A:243:ILE:HG22	1:A:243:ILE:O	2.05	0.56
1:A:40:ILE:O	3:A:705:PEG:H22	2.04	0.56
1:D:535:LEU:HD23	1:D:570:ILE:CD1	2.31	0.56
1:B:15:GLU:OE2	1:B:505:LYS:NZ	2.35	0.56
1:A:504:HIS:CD2	1:A:505:LYS:HG3	2.41	0.56
1:C:305:GLU:HG2	4:C:843:HOH:O	2.06	0.56
1:D:249:ASP:HB2	3:D:706:PEG:C3	2.36	0.55
1:D:379:GLU:N	1:D:380:PRO:HD2	2.21	0.55
1:D:331:PHE:HE2	1:D:354:LEU:HD22	1.70	0.55
1:D:202:LEU:HD11	1:D:206:LEU:HD11	1.89	0.55
1:D:472:ASP:OD1	1:D:476:ARG:HD2	2.07	0.55
1:D:111:GLN:NE2	1:D:490:HIS:HE1	2.05	0.55
1:B:3:ILE:N	1:B:3:ILE:HD12	2.21	0.55
1:C:271:ASP:C	1:C:271:ASP:OD1	2.45	0.55
1:C:302:ASN:H	1:C:302:ASN:HD22	1.55	0.54
1:D:99:ASP:CG	3:D:702:PEG:H42	2.27	0.54
1:A:92:LYS:HB3	3:A:706:PEG:H31	1.89	0.54
1:C:163:SER:O	4:C:852:HOH:O	2.18	0.54
1:A:563:TYR:CZ	1:A:594:ARG:HD3	2.42	0.54
1:C:202:LEU:HD23	1:C:202:LEU:O	2.08	0.54
1:B:137:THR:HG22	3:B:704:PEG:C1	2.31	0.54
1:B:535:LEU:HD23	1:B:570:ILE:HD13	1.90	0.54
1:D:33:PRO:HB3	1:D:465:ARG:HD3	1.90	0.54
1:A:563:TYR:CE1	1:A:594:ARG:HD3	2.43	0.54
3:B:704:PEG:C4	4:B:899:HOH:O	2.52	0.54
1:D:92:LYS:HD3	3:D:703:PEG:O1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLU:O	1:B:247:LYS:HB2	2.07	0.53
1:A:133:ARG:HD3	4:A:918:HOH:O	2.07	0.53
1:D:421:THR:HG23	1:D:424:GLN:OE1	2.07	0.53
1:D:268:VAL:C	1:D:270:SER:H	2.12	0.53
1:A:89:SER:HA	3:A:706:PEG:H42	1.91	0.53
1:B:590:ARG:HD2	4:B:888:HOH:O	2.07	0.53
1:B:149:GLU:HG2	3:B:703:PEG:H41	1.81	0.53
1:C:271:ASP:OD1	1:C:273:GLN:HG2	2.08	0.53
1:D:329:SER:OG	1:D:400:GLU:OE2	2.20	0.53
1:B:439:ILE:C	1:B:439:ILE:HD12	2.29	0.53
1:C:226:ARG:NH2	1:C:315:ASP:OD1	2.42	0.53
1:B:250:GLU:O	1:B:254:GLU:HG2	2.09	0.52
1:B:75:GLU:OE2	1:B:78:ARG:NH2	2.39	0.52
1:D:379:GLU:OE1	1:D:383:THR:HG22	2.09	0.52
1:A:15:GLU:OE2	1:A:505:LYS:CE	2.57	0.52
1:B:364:THR:HG23	1:B:455:LYS:HD2	1.90	0.52
1:D:580:ILE:HG23	1:D:584:GLN:HE21	1.74	0.52
1:A:134:GLN:CG	4:A:877:HOH:O	2.58	0.52
1:B:536:LEU:HD11	1:B:574:LEU:HD13	1.90	0.52
1:C:271:ASP:CG	1:C:273:GLN:HG2	2.30	0.52
1:A:472:ASP:OD1	1:A:476:ARG:HD2	2.10	0.52
1:C:202:LEU:HD23	1:C:206:LEU:CD1	2.39	0.52
3:B:704:PEG:C2	4:B:898:HOH:O	2.35	0.52
1:D:249:ASP:HB2	3:D:706:PEG:H41	1.92	0.52
1:A:16:ARG:O	3:A:702:PEG:C4	2.56	0.52
1:C:160:VAL:HG21	1:C:360:ILE:HD11	1.92	0.52
1:A:160:VAL:HG11	1:A:356:ALA:HB1	1.91	0.51
1:C:202:LEU:HD21	1:C:206:LEU:HD11	1.91	0.51
1:A:186:LYS:O	1:A:192:ARG:HA	2.09	0.51
1:A:560:TYR:O	1:A:564:ASN:HB2	2.10	0.51
1:C:160:VAL:HG22	1:C:178:PHE:HB3	1.93	0.51
1:B:133:ARG:CG	3:B:704:PEG:H32	2.41	0.51
1:C:91:LYS:NZ	1:C:99:ASP:OD1	2.43	0.51
1:C:246:GLU:O	1:C:247:LYS:HB2	2.10	0.51
1:C:202:LEU:HD12	1:C:376:PHE:HB3	1.92	0.51
1:C:401:PRO:O	1:C:405:ASP:N	2.25	0.51
1:B:137:THR:HB	3:B:704:PEG:H11	1.92	0.51
1:D:63:GLY:HA2	4:D:877:HOH:O	2.10	0.51
1:A:42:LEU:HD11	3:A:705:PEG:C1	2.41	0.50
1:B:243:ILE:HD12	1:B:306:ILE:CD1	2.41	0.50
1:C:27:LYS:HA	1:C:111:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ASN:ND2	1:D:455:LYS:NZ	2.59	0.50
1:B:579:SER:HB2	1:B:580:ILE:HD13	1.92	0.50
1:C:186:LYS:O	1:C:192:ARG:HA	2.12	0.50
1:C:271:ASP:OD2	1:C:273:GLN:HG2	2.12	0.50
1:C:357:GLU:HG3	1:C:432:PHE:HA	1.94	0.50
1:C:111:GLN:NE2	1:C:490:HIS:HE1	2.09	0.50
1:D:379:GLU:OE1	1:D:379:GLU:O	2.29	0.50
1:D:22:VAL:CG1	1:D:508:VAL:HG11	2.42	0.50
1:B:282:ASP:OD2	1:B:282:ASP:C	2.50	0.50
1:D:543:SER:HB2	1:D:544:PRO:HD2	1.93	0.50
1:B:15:GLU:CD	1:B:505:LYS:HZ3	2.13	0.50
1:B:157:ALA:HB3	1:B:459:ILE:HD12	1.94	0.50
1:C:6:VAL:HG12	1:C:8:VAL:HG12	1.94	0.50
1:C:329:SER:OG	1:C:400:GLU:OE2	2.27	0.49
1:D:345:ASP:O	1:D:349:ILE:HG12	2.12	0.49
1:B:472:ASP:OD1	1:B:476:ARG:HD2	2.13	0.49
1:D:260:GLN:NE2	1:D:279:LEU:H	2.10	0.49
1:D:260:GLN:HE21	1:D:279:LEU:H	1.59	0.49
1:D:186:LYS:O	1:D:192:ARG:HA	2.13	0.49
1:C:210:LEU:HD22	1:C:338:ILE:CD1	2.43	0.49
1:A:92:LYS:HE3	3:A:706:PEG:H32	1.88	0.49
1:D:246:GLU:HA	3:D:706:PEG:HO1	1.68	0.49
1:B:160:VAL:CG2	1:B:356:ALA:HB1	2.43	0.48
1:D:160:VAL:HG21	1:D:360:ILE:HD11	1.95	0.48
1:A:357:GLU:HG3	1:A:432:PHE:HA	1.95	0.48
1:A:530:ASN:O	1:A:532:PRO:HD3	2.12	0.48
1:C:331:PHE:HE2	1:C:354:LEU:HD22	1.77	0.48
1:D:75:GLU:OE2	1:D:78:ARG:NE	2.42	0.48
1:A:88:ASN:O	3:A:706:PEG:O2	2.31	0.48
1:B:23:ASP:OD2	1:B:29:HIS:HE1	1.97	0.48
1:A:157:ALA:HB3	1:A:459:ILE:HD12	1.95	0.48
1:A:89:SER:CA	3:A:706:PEG:H41	2.37	0.48
1:C:379:GLU:N	1:C:380:PRO:HD2	2.29	0.48
1:C:33:PRO:HB3	1:C:465:ARG:HD3	1.95	0.48
1:B:260:GLN:O	1:B:264:VAL:HG23	2.12	0.48
1:B:540:VAL:HG11	1:B:580:ILE:HD12	1.96	0.48
1:C:354:LEU:HD21	1:C:400:GLU:HA	1.95	0.48
1:A:133:ARG:CD	4:A:918:HOH:O	2.62	0.48
1:A:38:ASP:N	3:A:705:PEG:H21	2.17	0.47
1:A:40:ILE:HG22	3:A:705:PEG:H42	1.96	0.47
1:A:333:ASP:O	1:B:334:GLY:HA3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ILE:O	1:C:389:VAL:HG23	2.14	0.47
1:B:360:ILE:O	1:B:364:THR:HB	2.14	0.47
1:D:533:LYS:CE	4:D:901:HOH:O	2.63	0.47
1:A:184:ILE:HB	1:A:196:ILE:HB	1.95	0.47
1:A:359:ASN:ND2	1:A:372:PHE:H	2.13	0.47
1:B:134:GLN:OE1	4:B:897:HOH:O	2.20	0.47
1:B:338:ILE:CD1	1:B:347:ILE:HD13	2.45	0.47
1:C:243:ILE:N	1:C:243:ILE:HD12	2.30	0.47
1:D:20:LEU:CD1	1:D:28:VAL:HG13	2.45	0.47
1:C:535:LEU:CD2	1:C:570:ILE:HD13	2.41	0.46
1:D:357:GLU:HG3	1:D:432:PHE:HA	1.97	0.46
1:D:379:GLU:CD	1:D:379:GLU:O	2.54	0.46
1:B:476:ARG:HB3	3:B:703:PEG:C3	2.44	0.46
1:B:76:TYR:CD1	1:B:112:ILE:HD13	2.51	0.46
1:D:249:ASP:HB2	3:D:706:PEG:C4	2.45	0.46
1:D:529:GLU:O	1:D:530:ASN:C	2.53	0.46
1:A:439:ILE:HD12	1:A:439:ILE:C	2.36	0.46
1:B:535:LEU:HD23	1:B:570:ILE:CD1	2.45	0.46
1:D:179:ASN:HB3	1:D:371:ASN:HD21	1.80	0.46
1:A:138:GLY:O	1:B:284:ARG:CZ	2.64	0.46
1:A:342:ARG:N	1:A:342:ARG:HD2	2.30	0.46
1:A:8:VAL:O	1:A:8:VAL:HG13	2.15	0.46
1:C:164:PRO:HA	1:C:349:ILE:HD11	1.97	0.46
1:C:455:LYS:HG2	1:C:456:LYS:H	1.80	0.46
1:C:371:ASN:OD1	1:C:373:GLY:N	2.49	0.46
1:B:114:LYS:NZ	1:B:486:ASP:HB2	2.32	0.45
1:C:421:THR:HG23	1:C:424:GLN:OE1	2.17	0.45
1:C:260:GLN:NE2	1:C:279:LEU:H	2.14	0.45
3:A:706:PEG:H12	4:A:914:HOH:O	2.15	0.45
1:D:540:VAL:HG21	1:D:580:ILE:HD13	1.97	0.45
1:D:89:SER:HA	3:D:703:PEG:H12	1.98	0.45
1:C:179:ASN:HB3	1:C:371:ASN:HD21	1.82	0.45
1:D:164:PRO:HA	1:D:349:ILE:HD11	1.98	0.45
1:D:408:ASN:C	1:D:410:ASN:H	2.20	0.45
1:D:474:PHE:CZ	1:D:478:THR:HG21	2.52	0.45
1:D:6:VAL:HG12	1:D:8:VAL:HG12	1.98	0.45
1:A:282:ASP:OD2	1:A:283:PRO:CD	2.62	0.44
1:D:122:LEU:HD21	1:D:473:PHE:HE2	1.81	0.44
1:B:93:ILE:HG23	1:B:600:ASP:HB3	1.99	0.44
1:C:294:VAL:O	1:C:298:MET:HA	2.18	0.44
1:D:178:PHE:C	1:D:178:PHE:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASP:C	1:D:214:ASP:OD1	2.56	0.44
1:B:184:ILE:HB	1:B:196:ILE:HB	2.00	0.44
1:C:228:LYS:HZ2	1:C:266:GLU:CD	2.21	0.44
1:C:498:THR:O	1:C:498:THR:HG22	2.16	0.44
1:A:219:PRO:HG2	1:A:394:THR:HG22	2.00	0.44
1:A:42:LEU:HD11	3:A:705:PEG:H11	2.00	0.44
1:B:31:LEU:HD22	1:B:31:LEU:N	2.31	0.44
1:B:114:LYS:HB2	1:B:487:LEU:HD11	2.00	0.44
1:C:472:ASP:OD1	1:C:476:ARG:HD2	2.18	0.44
1:C:508:VAL:HG23	4:C:842:HOH:O	2.18	0.44
1:A:330:PRO:HD3	1:A:433:THR:HG23	1.99	0.44
1:B:137:THR:HG21	3:B:704:PEG:C1	2.22	0.44
1:B:508:VAL:HG23	4:B:858:HOH:O	2.17	0.44
1:C:121:VAL:CG2	1:C:125:GLN:OE1	2.66	0.44
1:D:536:LEU:HA	1:D:536:LEU:HD12	1.74	0.43
1:A:20:LEU:CD2	1:A:22:VAL:HG23	2.48	0.43
1:C:284:ARG:NH1	1:D:138:GLY:O	2.48	0.43
1:D:191:SER:O	1:D:192:ARG:HB2	2.18	0.43
1:D:354:LEU:HD21	1:D:400:GLU:HA	1.99	0.43
1:B:15:GLU:OE1	4:B:870:HOH:O	2.21	0.43
1:B:182:ARG:NE	3:B:702:PEG:H22	2.26	0.43
1:C:179:ASN:O	1:C:373:GLY:HA3	2.19	0.43
1:D:91:LYS:NZ	1:D:99:ASP:OD1	2.51	0.43
1:B:332:TYR:OH	1:B:397:ALA:O	2.28	0.43
1:B:238:LYS:N	1:B:241:ASP:OD2	2.52	0.43
1:C:360:ILE:O	1:C:364:THR:HB	2.18	0.43
1:C:439:ILE:C	1:C:439:ILE:CD1	2.87	0.43
1:D:111:GLN:HE21	1:D:490:HIS:CE1	2.37	0.43
1:B:587:ASP:OD1	1:B:590:ARG:NH2	2.52	0.43
1:A:243:ILE:CD1	1:A:243:ILE:N	2.82	0.43
1:A:76:TYR:CD1	1:A:112:ILE:HD13	2.54	0.43
1:C:202:LEU:HD23	1:C:202:LEU:C	2.39	0.43
1:D:91:LYS:NZ	3:D:702:PEG:O2	2.47	0.43
1:B:229:VAL:O	1:B:233:VAL:HG23	2.19	0.43
1:C:214:ASP:OD1	1:C:214:ASP:C	2.57	0.43
1:D:184:ILE:HB	1:D:196:ILE:HB	2.01	0.43
1:D:365:ASN:HD21	1:D:455:LYS:HZ3	1.65	0.43
1:C:535:LEU:HD23	1:C:570:ILE:CD1	2.40	0.42
1:B:31:LEU:CD2	1:B:31:LEU:N	2.82	0.42
1:B:590:ARG:NE	4:B:888:HOH:O	2.51	0.42
1:C:300:VAL:HG22	1:C:304:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:HD23	3:D:702:PEG:H41	2.02	0.42
1:A:14:PRO:HG3	3:A:702:PEG:O2	2.20	0.42
1:D:99:ASP:OD1	3:D:702:PEG:C4	2.66	0.42
1:D:33:PRO:HB2	1:D:51:GLU:HB3	2.00	0.42
1:A:204:TYR:CE1	1:A:208:SER:HB3	2.54	0.42
1:B:234:LEU:HA	1:B:234:LEU:HD23	1.91	0.42
1:B:33:PRO:HB3	1:B:465:ARG:HD3	2.02	0.42
1:C:202:LEU:CD2	1:C:206:LEU:HD11	2.47	0.42
1:D:365:ASN:ND2	1:D:455:LYS:HZ3	2.18	0.42
1:A:33:PRO:HB3	1:A:465:ARG:HD3	2.01	0.42
1:C:410:ASN:O	1:C:411:HIS:C	2.58	0.42
1:D:215:LYS:O	1:D:217:PRO:HD3	2.19	0.42
1:D:294:VAL:O	1:D:298:MET:HA	2.19	0.42
1:D:408:ASN:O	1:D:410:ASN:N	2.52	0.42
1:D:250:GLU:HG3	3:D:706:PEG:H42	2.00	0.42
1:B:465:ARG:HH21	3:B:705:PEG:C3	2.29	0.42
1:C:560:TYR:O	1:C:564:ASN:HB2	2.20	0.42
1:D:282:ASP:HB2	1:D:283:PRO:HD2	2.02	0.42
1:B:399:ILE:HA	1:B:402:ILE:HD12	2.01	0.42
1:B:566:ASN:O	1:B:569:ALA:HB3	2.20	0.42
1:C:178:PHE:C	1:C:178:PHE:CD1	2.93	0.42
1:B:118:LEU:O	1:B:121:VAL:HG12	2.20	0.41
1:D:248:LYS:HG2	3:D:706:PEG:H22	2.02	0.41
1:C:77:LYS:HG3	1:C:109:LEU:HD11	2.02	0.41
1:D:248:LYS:N	3:D:706:PEG:H22	2.36	0.41
1:A:246:GLU:OE2	1:A:246:GLU:HA	2.20	0.41
1:A:91:LYS:NZ	1:A:99:ASP:OD1	2.54	0.41
1:C:204:TYR:CE1	1:C:208:SER:HB3	2.55	0.41
1:C:282:ASP:HB2	1:C:283:PRO:HD2	2.02	0.41
1:A:283:PRO:C	1:A:285:GLY:H	2.24	0.41
1:D:357:GLU:OE2	1:D:435:HIS:ND1	2.32	0.41
1:D:554:SER:O	1:D:555:LYS:C	2.59	0.41
1:B:238:LYS:O	1:B:240:GLU:N	2.54	0.41
1:D:400:GLU:N	1:D:401:PRO:CD	2.84	0.41
1:B:580:ILE:HA	1:B:581:PRO:HD2	1.91	0.41
1:B:66:LYS:HE2	3:B:705:PEG:H41	2.02	0.41
1:C:229:VAL:O	1:C:233:VAL:HG23	2.20	0.41
1:A:243:ILE:N	1:A:243:ILE:HD12	2.36	0.41
1:A:472:ASP:O	1:A:476:ARG:HG3	2.21	0.41
1:B:306:ILE:O	1:B:310:ILE:HG13	2.21	0.41
1:D:268:VAL:HG13	1:D:269:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ARG:HB3	3:B:703:PEG:H32	2.02	0.40
1:B:590:ARG:CD	4:B:888:HOH:O	2.67	0.40
1:C:75[A]:GLU:OE1	1:C:78:ARG:HD2	2.21	0.40
1:D:431:LYS:HE3	4:D:859:HOH:O	2.21	0.40
1:A:294:VAL:HG22	1:A:300:VAL:O	2.21	0.40
1:B:56:PHE:O	1:B:123:LYS:NZ	2.54	0.40
1:D:400:GLU:HB2	1:D:401:PRO:HD3	2.03	0.40
1:A:103:LYS:HE2	4:A:895:HOH:O	2.21	0.40
1:C:561:ILE:HG21	1:C:592:LEU:HD13	2.03	0.40
1:A:349:ILE:HA	1:A:349:ILE:HD13	1.86	0.40
1:A:42:LEU:HD11	3:A:705:PEG:H12	2.03	0.40
1:D:447:GLU:HG3	4:D:876:HOH:O	2.20	0.40
1:D:543:SER:HB2	1:D:544:PRO:CD	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ASN:O	3:A:706:PEG:O1[1_655]	2.01	0.19

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	603/611 (99%)	580 (96%)	23 (4%)	0	100	100
1	B	606/611 (99%)	580 (96%)	25 (4%)	1 (0%)	51	67
1	C	610/611 (100%)	576 (94%)	33 (5%)	1 (0%)	51	67
1	D	609/611 (100%)	568 (93%)	38 (6%)	3 (0%)	32	46
All	All	2428/2444 (99%)	2304 (95%)	119 (5%)	5 (0%)	51	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	269	LYS
1	D	409	SER
1	D	139	GLY
1	B	3	ILE
1	C	0	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	530/554 (96%)	519 (98%)	11 (2%)	59	78
1	B	534/554 (96%)	520 (97%)	14 (3%)	51	72
1	C	537/554 (97%)	522 (97%)	15 (3%)	49	70
1	D	538/554 (97%)	527 (98%)	11 (2%)	60	79
All	All	2139/2216 (96%)	2088 (98%)	51 (2%)	54	74

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	250	GLU
1	A	268	VAL
1	A	283	PRO
1	A	302	ASN
1	A	342	ARG
1	A	385	ILE
1	A	517	ASP
1	A	536	LEU
1	A	540	VAL
1	A	565	ARG
1	B	64	VAL
1	B	121	VAL
1	B	131	ASP
1	B	136	ARG
1	B	250	GLU
1	B	268	VAL

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Mol	Chain	Res	Type
1	B	280	SER
1	B	364	THR
1	B	409	SER
1	B	483	PRO
1	B	498	THR
1	B	517	ASP
1	B	578	THR
1	B	579	SER
1	C	140	ILE
1	C	160	VAL
1	C	224	SER
1	C	240	GLU
1	C	281	LYS
1	C	298	MET
1	C	300	VAL
1	C	302	ASN
1	C	305	GLU
1	C	359	ASN
1	C	364	THR
1	C	536	LEU
1	C	570	ILE
1	C	578	THR
1	C	587	ASP
1	D	121	VAL
1	D	160	VAL
1	D	231	SER
1	D	277	LEU
1	D	324	VAL
1	D	359	ASN
1	D	364	THR
1	D	418	SER
1	D	479	LYS
1	D	517	ASP
1	D	597	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	134	GLN
1	A	359	ASN
1	B	29	HIS

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Mol	Chain	Res	Type
1	B	359	ASN
1	B	395	GLN
1	B	584	GLN
1	C	111	GLN
1	C	260	GLN
1	C	302	ASN
1	C	490	HIS
1	D	111	GLN
1	D	260	GLN
1	D	365	ASN
1	D	490	HIS
1	D	564	ASN
1	D	584	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\# Z > 2$
3	PEG	A	702	-	6,6,6	0.71	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	703	-	6,6,6	0.76	0	5,5,5	0.59	0
3	PEG	A	704	-	6,6,6	1.13	0	5,5,5	1.25	1 (20%)
3	PEG	A	705	-	6,6,6	0.58	0	5,5,5	0.86	0
3	PEG	A	706	-	6,6,6	0.52	0	5,5,5	0.64	0
3	PEG	A	707	-	6,6,6	0.70	0	5,5,5	0.26	0
3	PEG	B	702	-	6,6,6	0.36	0	5,5,5	1.47	1 (20%)
3	PEG	B	703	-	6,6,6	0.79	0	5,5,5	1.18	0
3	PEG	B	704	-	6,6,6	0.53	0	5,5,5	1.11	0
3	PEG	B	705	-	6,6,6	0.67	0	5,5,5	0.87	0
3	PEG	C	702	-	6,6,6	0.87	0	5,5,5	1.10	0
3	PEG	C	703	-	6,6,6	0.63	0	5,5,5	0.96	0
3	PEG	D	702	-	6,6,6	0.96	0	5,5,5	1.09	0
3	PEG	D	703	-	6,6,6	0.81	0	5,5,5	0.29	0
3	PEG	D	704	-	6,6,6	0.78	0	5,5,5	0.43	0
3	PEG	D	705	-	6,6,6	0.60	0	5,5,5	0.31	0
3	PEG	D	706	-	6,6,6	0.52	0	5,5,5	0.58	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
3	PEG	A	702	-	-	0/4/4/4	0/0/0/0
3	PEG	A	703	-	-	0/4/4/4	0/0/0/0
3	PEG	A	704	-	-	0/4/4/4	0/0/0/0
3	PEG	A	705	-	-	0/4/4/4	0/0/0/0
3	PEG	A	706	-	-	0/4/4/4	0/0/0/0
3	PEG	A	707	-	-	0/4/4/4	0/0/0/0
3	PEG	B	702	-	-	0/4/4/4	0/0/0/0
3	PEG	B	703	-	-	0/4/4/4	0/0/0/0
3	PEG	B	704	-	-	0/4/4/4	0/0/0/0
3	PEG	B	705	-	-	0/4/4/4	0/0/0/0
3	PEG	C	702	-	-	0/4/4/4	0/0/0/0
3	PEG	C	703	-	-	0/4/4/4	0/0/0/0
3	PEG	D	702	-	-	0/4/4/4	0/0/0/0
3	PEG	D	703	-	-	0/4/4/4	0/0/0/0
3	PEG	D	704	-	-	0/4/4/4	0/0/0/0
3	PEG	D	705	-	-	0/4/4/4	0/0/0/0
3	PEG	D	706	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	PEG	C3-O2-C2	-2.46	102.65	113.30
3	A	704	PEG	O1-C1-C2	2.14	124.16	111.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	PEG	3	0
3	A	703	PEG	1	0
3	A	705	PEG	12	0
3	A	706	PEG	11	1
3	B	702	PEG	2	0
3	B	703	PEG	6	0
3	B	704	PEG	17	0
3	B	705	PEG	3	0
3	C	703	PEG	1	0
3	D	702	PEG	5	0
3	D	703	PEG	2	0
3	D	706	PEG	13	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 [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, 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	604/611 (98%)	-0.44	1 (0%) 94 94	32, 46, 70, 86	0
1	B	608/611 (99%)	-0.44	0 100 100	31, 46, 70, 88	0
1	C	611/611 (100%)	-0.40	1 (0%) 94 94	34, 52, 69, 78	0
1	D	610/611 (99%)	-0.38	1 (0%) 94 94	34, 51, 69, 77	0
All	All	2433/2444 (99%)	-0.42	3 (0%) 95 95	31, 49, 69, 88	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	PRO	3.0
1	C	420	LEU	2.2
1	A	6	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PEG	A	702	7/7	0.87	0.27	11.43	59,64,69,71	0
3	PEG	C	703	7/7	0.87	0.19	4.55	54,58,62,63	0
3	PEG	A	704	7/7	0.84	0.21	4.45	43,54,59,61	0
3	PEG	A	703	7/7	0.91	0.25	3.63	37,44,50,52	0
3	PEG	A	705	7/7	0.87	0.19	3.00	43,48,54,57	0
3	PEG	A	706	7/7	0.94	0.18	2.87	67,68,71,71	0
3	PEG	D	702	7/7	0.94	0.21	2.54	44,54,57,58	0
3	PEG	D	703	7/7	0.89	0.17	2.39	70,73,75,75	0
2	MG	A	701	1/1	0.95	0.17	2.34	63,63,63,63	0
3	PEG	D	705	7/7	0.94	0.18	1.71	66,67,69,69	0
3	PEG	B	702	7/7	0.96	0.16	1.18	46,47,49,51	0
3	PEG	C	702	7/7	0.93	0.17	0.83	48,53,60,60	0
3	PEG	D	706	7/7	0.88	0.17	0.46	74,74,76,76	0
2	MG	D	701	1/1	0.97	0.12	-0.15	65,65,65,65	0
2	MG	B	701	1/1	0.94	0.12	-0.15	70,70,70,70	0
3	PEG	A	707	7/7	0.85	0.13	-0.25	72,77,82,82	0
2	MG	C	701	1/1	0.97	0.12	-0.55	62,62,62,62	0
3	PEG	B	705	7/7	0.92	0.12	-0.74	68,69,72,72	0
3	PEG	B	703	7/7	0.84	0.26	-	63,65,69,72	0
3	PEG	B	704	7/7	0.82	0.16	-	69,70,72,72	0
3	PEG	D	704	7/7	0.76	0.17	-	61,66,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.