



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:36 AM GMT

PDB ID : 3PFL
Title : CRYSTAL STRUCTURE OF PFL FROM E.COLI IN COMPLEX WITH
SUBSTRATE ANALOGUE OXAMATE
Authors : Becker, A.; Fritz-Wolf, K.; Kabsch, W.; Knappe, J.; Schultz, S.; Wagner,
A.F.V.
Deposited on : 1999-05-14
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

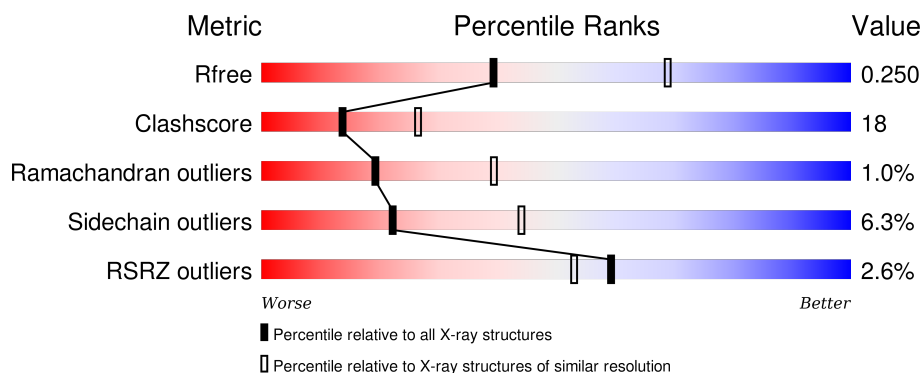
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 ≥ 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	759	<div> <div>2%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	B	759	<div> <div>3%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>

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
2	OXM	A	761	-	-	-	X

2 Entry composition [i](#)

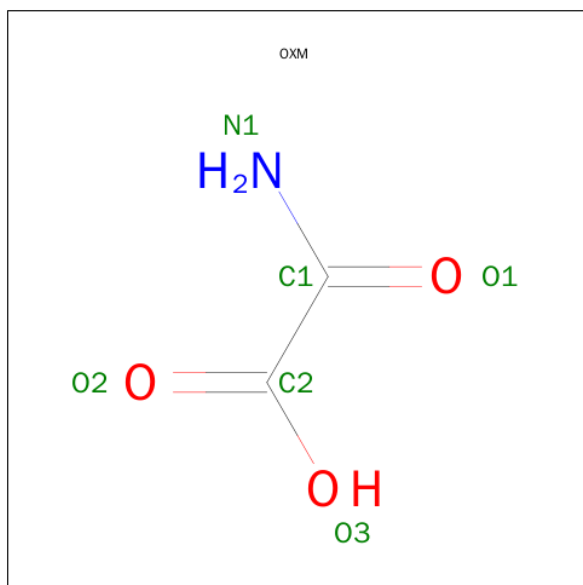
There are 3 unique types of molecules in this entry. The entry contains 12515 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (FORMATE ACETYLTRANSFERASE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			5988	3784	1023	1145	36			
1	B	759	Total	C	N	O	S	0	0	0
			5988	3784	1023	1145	36			

- Molecule 2 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	2	1	3		
2	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	294	Total 294	O 294	0	0
3	B	233	Total 233	O 233	0	0

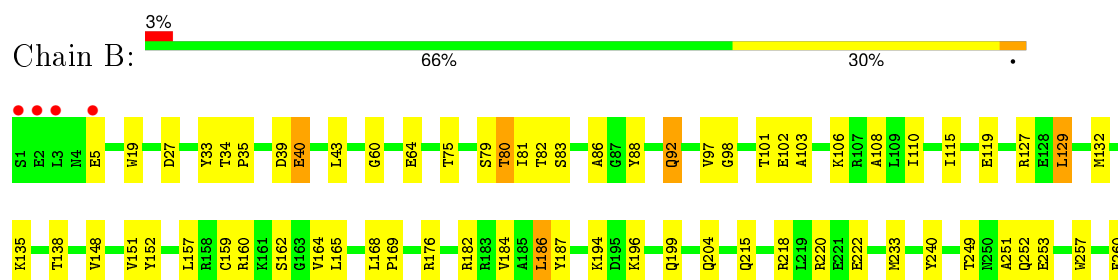
3 Residue-property plots

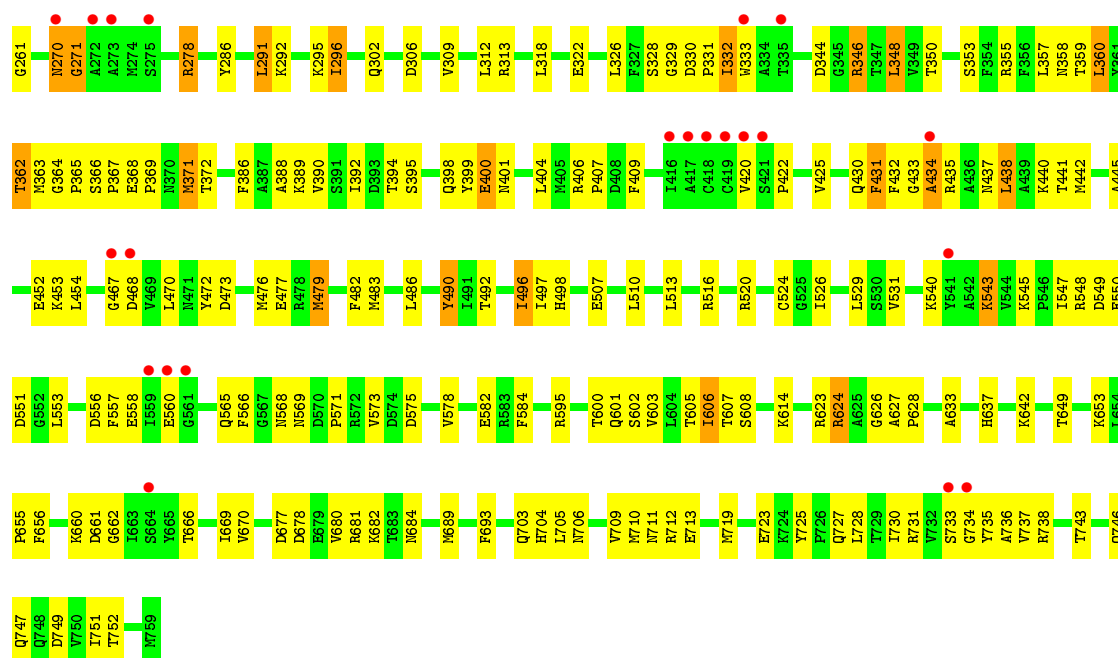
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: PROTEIN (FORMATE ACETYLTRANSFERASE 1)



• Molecule 1: PROTEIN (FORMATE ACETYLTRANSFERASE 1)





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.21Å 159.21Å 160.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.60) 96.2 (48.03-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.61Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.212 , 0.251 0.212 , 0.250	Depositor DCC
R_{free} test set	2927 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.4	EDS
Estimated twinning fraction	0.017 for -h,l,k 0.005 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61282 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12515	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	0/6109	0.61	0/8253
1	B	0.43	0/6109	0.61	0/8253
All	All	0.42	0/12218	0.61	0/16506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5988	0	5914	211	0
1	B	5988	0	5914	232	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
3	A	294	0	0	12	0
3	B	233	0	0	13	0
All	All	12515	0	11832	440	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 (440) 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:332:ILE:HB	3:B:951:HOH:O	1.45	1.12
1:A:602:SER:HB3	1:A:661:ASP:HB3	1.40	1.03
1:B:602:SER:HB3	1:B:661:ASP:HB3	1.43	0.97
1:B:362:THR:HG23	1:B:363:MET:HG3	1.47	0.97
1:A:614:LYS:HA	1:A:626:GLY:HA2	1.47	0.96
1:B:614:LYS:HA	1:B:626:GLY:HA2	1.48	0.93
1:A:362:THR:HG23	1:A:363:MET:HG3	1.50	0.92
1:A:712:ARG:NH1	1:A:751:ILE:HG22	1.88	0.89
1:B:712:ARG:NH1	1:B:751:ILE:HG22	1.88	0.88
1:A:712:ARG:HH11	1:A:751:ILE:HG22	1.41	0.86
1:B:712:ARG:HH11	1:B:751:ILE:HG22	1.40	0.85
1:A:101:THR:HG21	1:A:106:LYS:HB3	1.58	0.85
1:B:101:THR:HG21	1:B:106:LYS:HB3	1.58	0.84
1:A:670:VAL:HG13	1:A:711:ASN:HD21	1.41	0.84
1:A:359:THR:HA	1:A:362:THR:HG22	1.60	0.83
1:A:182:ARG:NH2	1:A:425:VAL:HG21	1.94	0.83
1:B:359:THR:HA	1:B:362:THR:HG22	1.61	0.82
1:A:406:ARG:HB3	1:A:407:PRO:HD3	1.62	0.82
1:B:182:ARG:NH2	1:B:425:VAL:HG21	1.95	0.81
1:B:40:GLU:HG2	1:B:386:PHE:CD1	2.15	0.81
1:B:606:ILE:HG22	1:B:607:THR:H	1.44	0.81
1:A:40:GLU:HG2	1:A:386:PHE:CD1	2.17	0.80
1:B:406:ARG:HB3	1:B:407:PRO:HD3	1.63	0.80
1:B:34:THR:HG23	3:B:799:HOH:O	1.81	0.80
1:A:606:ILE:HG22	1:A:607:THR:H	1.47	0.79
1:A:689:MET:HE3	1:A:705:LEU:HD23	1.65	0.79
1:B:438:LEU:HD21	1:B:483:MET:HE2	1.65	0.78
1:B:101:THR:HG23	1:B:103:ALA:H	1.47	0.78
1:A:670:VAL:HG13	1:A:711:ASN:ND2	1.99	0.77
1:B:92:GLN:NE2	1:B:92:GLN:H	1.82	0.77
1:A:101:THR:HG23	1:A:103:ALA:H	1.49	0.77
1:B:543:LYS:HB2	1:B:560:GLU:HB3	1.66	0.77
1:B:689:MET:HE3	1:B:705:LEU:HD23	1.67	0.77
1:A:92:GLN:NE2	1:A:92:GLN:H	1.82	0.76
1:A:4:ASN:HD22	1:A:6:LYS:H	1.29	0.76
1:B:600:THR:HG22	1:B:661:ASP:HB2	1.66	0.76
1:A:4:ASN:H	1:A:7:LEU:HD12	1.51	0.75
1:A:80:THR:HG22	1:A:82:THR:H	1.51	0.74
1:B:80:THR:HG22	1:B:82:THR:H	1.51	0.74
1:A:600:THR:HG22	1:A:661:ASP:HB2	1.68	0.74
1:B:545:LYS:HB3	1:B:558:GLU:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:HG2	3:B:901:HOH:O	1.87	0.73
1:A:4:ASN:HB3	1:A:7:LEU:HG	1.72	0.72
1:A:4:ASN:ND2	1:A:6:LYS:H	1.88	0.71
1:B:670:VAL:HG13	1:B:711:ASN:HD21	1.55	0.71
1:A:725:TYR:HB3	1:A:728:LEU:HB2	1.73	0.70
1:B:725:TYR:HB3	1:B:728:LEU:HB2	1.74	0.70
1:A:278:ARG:HD2	3:A:925:HOH:O	1.92	0.70
1:B:182:ARG:HH22	1:B:425:VAL:HG21	1.57	0.69
1:A:719:MET:SD	1:A:751:ILE:HD11	2.32	0.69
1:A:689:MET:CE	1:A:705:LEU:HD23	2.22	0.69
1:A:389:LYS:HG2	1:A:682:LYS:HD3	1.75	0.68
1:A:182:ARG:HH22	1:A:425:VAL:HG21	1.59	0.68
1:B:101:THR:HG22	3:B:807:HOH:O	1.92	0.68
1:A:743:THR:O	1:A:747:GLN:HG3	1.95	0.67
1:B:399:TYR:CD1	1:B:689:MET:HE1	2.29	0.67
1:B:719:MET:SD	1:B:751:ILE:HD11	2.34	0.67
1:A:364:GLY:HA3	1:A:727:GLN:HE22	1.60	0.67
1:B:389:LYS:HG2	1:B:682:LYS:HD3	1.77	0.67
1:A:677:ASP:OD1	1:A:680:VAL:HG23	1.95	0.66
1:B:547:ILE:HB	1:B:556:ASP:HB3	1.76	0.66
1:A:545:LYS:HG2	1:A:558:GLU:HB2	1.76	0.66
1:B:372:THR:HG23	1:B:398:GLN:HG3	1.78	0.66
1:A:80:THR:HB	1:A:83:SER:HB3	1.78	0.65
1:A:624:ARG:HG3	1:A:624:ARG:HH11	1.61	0.65
1:A:372:THR:HG23	1:A:398:GLN:HG3	1.77	0.65
1:A:399:TYR:CD1	1:A:689:MET:HE1	2.32	0.65
1:B:689:MET:CE	1:B:705:LEU:HD23	2.26	0.65
1:B:80:THR:HB	1:B:83:SER:HB3	1.78	0.65
1:B:710:MET:HE1	1:B:730:ILE:HG22	1.77	0.65
1:A:233:MET:CE	1:A:261:GLY:HA2	2.26	0.65
1:B:332:ILE:HG23	1:B:368:GLU:CD	2.17	0.65
1:A:332:ILE:HG23	1:A:368:GLU:CD	2.17	0.65
1:B:176:ARG:HH11	1:B:430:GLN:HE21	1.43	0.65
1:B:743:THR:O	1:B:747:GLN:HG3	1.96	0.65
1:B:680:VAL:HG12	1:B:684:ASN:ND2	2.11	0.65
1:B:680:VAL:HG12	1:B:684:ASN:HD21	1.62	0.65
1:B:40:GLU:HG2	1:B:386:PHE:CE1	2.32	0.65
1:B:566:PHE:N	1:B:573:VAL:HG21	2.12	0.64
1:B:364:GLY:HA3	1:B:727:GLN:HE22	1.62	0.64
1:B:220:ARG:NH2	3:B:873:HOH:O	2.25	0.64
1:A:151:VAL:O	1:B:220:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:MET:CE	1:B:261:GLY:HA2	2.28	0.64
1:A:359:THR:HA	1:A:362:THR:CG2	2.28	0.64
1:A:680:VAL:HG12	1:A:684:ASN:ND2	2.12	0.64
1:B:624:ARG:HG3	1:B:624:ARG:HH11	1.63	0.63
1:B:306:ASP:OD1	1:B:362:THR:HG21	1.99	0.63
1:B:438:LEU:HD21	1:B:483:MET:CE	2.28	0.63
1:A:666:THR:HA	1:A:706:ASN:HB2	1.81	0.62
1:A:680:VAL:HG12	1:A:684:ASN:HD21	1.64	0.62
1:A:115:ILE:HG21	1:A:138:THR:CG2	2.30	0.62
1:A:220:ARG:NH2	3:A:885:HOH:O	2.31	0.62
1:B:115:ILE:HG21	1:B:138:THR:CG2	2.30	0.62
1:A:40:GLU:HG2	1:A:386:PHE:CE1	2.34	0.61
1:A:578:VAL:O	1:A:582:GLU:HG3	2.01	0.61
1:B:578:VAL:O	1:B:582:GLU:HG3	2.01	0.61
1:B:332:ILE:HD12	3:B:831:HOH:O	2.01	0.61
1:A:306:ASP:OD1	1:A:362:THR:HG21	2.01	0.60
1:B:496:ILE:HG13	1:B:497:ILE:N	2.17	0.60
1:B:649:THR:HG22	1:B:653:LYS:HE3	1.83	0.60
1:B:359:THR:HA	1:B:362:THR:CG2	2.29	0.60
1:B:677:ASP:OD1	1:B:680:VAL:HG23	2.01	0.60
1:B:148:VAL:HG13	1:B:496:ILE:HD11	1.84	0.60
1:A:249:THR:HB	1:A:253:GLU:OE1	2.02	0.60
1:B:249:THR:HB	1:B:253:GLU:OE1	2.02	0.60
1:A:710:MET:HE3	1:A:730:ILE:HG22	1.84	0.60
1:A:148:VAL:HG13	1:A:496:ILE:HD11	1.82	0.59
1:B:600:THR:CG2	1:B:661:ASP:HB2	2.32	0.59
1:B:656:PHE:CD1	1:B:703:GLN:HG3	2.38	0.59
1:A:706:ASN:HD21	1:A:734:GLY:N	2.01	0.59
1:A:496:ILE:HG13	1:A:497:ILE:N	2.17	0.59
1:A:165:LEU:HD22	1:A:168:LEU:HD11	1.84	0.58
1:B:39:ASP:HB2	1:B:40:GLU:OE2	2.03	0.58
1:B:168:LEU:HD12	1:B:434:ALA:HB3	1.83	0.58
1:B:706:ASN:HD21	1:B:734:GLY:N	2.02	0.58
1:B:291:LEU:HD13	1:B:296:ILE:HG22	1.85	0.58
1:A:649:THR:O	1:A:653:LYS:HG3	2.03	0.58
1:A:291:LEU:HD13	1:A:296:ILE:HG22	1.84	0.58
1:B:409:PHE:HE2	1:B:422:PRO:HB2	1.69	0.58
1:B:492:THR:O	1:B:496:ILE:HG23	2.04	0.58
1:B:278:ARG:HD2	3:B:793:HOH:O	2.02	0.58
1:B:218:ARG:O	1:B:222:GLU:HG3	2.03	0.58
1:A:158:ARG:HG2	1:A:456:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PHE:CD1	1:A:703:GLN:HG3	2.38	0.58
1:A:218:ARG:O	1:A:222:GLU:HG3	2.04	0.58
1:A:39:ASP:HB2	1:A:40:GLU:OE2	2.04	0.57
1:A:678:ASP:O	1:A:682:LYS:HG3	2.04	0.57
1:B:176:ARG:HH11	1:B:430:GLN:NE2	2.03	0.57
1:B:565:GLN:O	1:B:573:VAL:HG11	2.04	0.57
1:B:132:MET:HE1	1:B:135:LYS:HD3	1.86	0.57
1:B:470:LEU:HD11	1:B:557:PHE:HE2	1.68	0.57
1:A:719:MET:SD	1:A:751:ILE:CD1	2.92	0.57
1:B:606:ILE:HG22	1:B:607:THR:N	2.18	0.57
1:A:433:GLY:O	1:A:434:ALA:O	2.23	0.57
1:B:176:ARG:HG3	1:B:432:PHE:HB2	1.87	0.57
1:B:565:GLN:C	1:B:573:VAL:HG11	2.25	0.57
1:A:220:ARG:NH1	1:B:151:VAL:O	2.37	0.57
1:A:409:PHE:HE2	1:A:422:PRO:HB2	1.68	0.56
1:A:328:SER:HB3	1:A:746:GLN:NE2	2.20	0.56
1:A:649:THR:HG22	1:A:653:LYS:HE3	1.87	0.56
1:B:719:MET:SD	1:B:751:ILE:CD1	2.94	0.56
1:A:80:THR:HG23	3:A:874:HOH:O	2.06	0.56
1:B:176:ARG:CG	1:B:432:PHE:HB2	2.35	0.56
1:A:289:ARG:HD2	3:A:1031:HOH:O	2.06	0.56
1:B:670:VAL:HG13	1:B:711:ASN:ND2	2.20	0.56
1:B:678:ASP:O	1:B:682:LYS:HG3	2.05	0.56
1:A:600:THR:CG2	1:A:661:ASP:HB2	2.36	0.55
1:A:670:VAL:HG13	1:A:671:PRO:HD2	1.87	0.55
1:A:80:THR:CG2	3:A:874:HOH:O	2.54	0.55
1:B:186:LEU:HD13	1:B:187:TYR:CE2	2.41	0.55
1:B:332:ILE:CG2	1:B:368:GLU:HG3	2.37	0.55
1:A:547:ILE:HD12	1:A:556:ASP:HB3	1.87	0.55
1:A:492:THR:O	1:A:496:ILE:HG23	2.06	0.55
1:B:470:LEU:HD11	1:B:557:PHE:CE2	2.42	0.55
1:A:344:ASP:OD1	1:A:346:ARG:HG2	2.07	0.54
1:B:420:VAL:HG23	1:B:662:GLY:HA3	1.88	0.54
1:B:313:ARG:HG2	1:B:368:GLU:O	2.06	0.54
1:A:353:SER:O	1:A:357:LEU:HD13	2.07	0.54
1:A:186:LEU:HD13	1:A:187:TYR:CE2	2.42	0.54
1:B:649:THR:O	1:B:653:LYS:HG3	2.07	0.54
1:B:549:ASP:OD1	1:B:553:LEU:HB3	2.07	0.54
1:B:490:TYR:CE2	1:B:524:CYS:HB3	2.42	0.54
1:A:420:VAL:HG23	1:A:662:GLY:HA3	1.89	0.54
1:B:313:ARG:CZ	1:B:366:SER:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:THR:CG2	1:B:400:GLU:HG3	2.38	0.54
1:B:353:SER:O	1:B:357:LEU:HD13	2.08	0.54
1:A:313:ARG:HG2	1:A:368:GLU:O	2.07	0.54
1:B:92:GLN:H	1:B:92:GLN:HE21	1.54	0.54
1:A:486:LEU:HD12	1:A:584:PHE:CZ	2.43	0.54
1:B:605:THR:O	1:B:608:SER:HB2	2.08	0.54
1:B:747:GLN:O	1:B:751:ILE:HG13	2.08	0.53
1:A:601:GLN:HG2	1:A:602:SER:N	2.24	0.53
1:A:602:SER:HB3	1:A:661:ASP:CB	2.27	0.53
1:A:313:ARG:CZ	1:A:366:SER:HB2	2.38	0.53
1:B:556:ASP:OD1	1:B:557:PHE:N	2.42	0.53
1:B:486:LEU:HD12	1:B:584:PHE:CZ	2.43	0.53
1:A:452:GLU:HA	1:A:553:LEU:HD21	1.90	0.53
1:A:115:ILE:HG21	1:A:138:THR:HG23	1.91	0.53
1:B:472:TYR:HD1	1:B:473:ASP:OD1	1.92	0.53
1:A:146:GLN:HG2	3:A:1019:HOH:O	2.08	0.53
1:B:520:ARG:NH1	3:B:790:HOH:O	2.40	0.53
1:B:194:LYS:HB3	1:B:194:LYS:NZ	2.24	0.53
1:B:601:GLN:HG2	1:B:602:SER:N	2.23	0.52
1:A:606:ILE:HG22	1:A:607:THR:N	2.19	0.52
1:B:40:GLU:H	1:B:40:GLU:CD	2.12	0.52
1:B:442:MET:HA	1:B:479:MET:HE3	1.90	0.52
1:B:437:ASN:ND2	1:B:440:LYS:HB2	2.25	0.52
1:A:4:ASN:ND2	1:A:5:GLU:N	2.58	0.52
1:B:215:GLN:CD	1:B:215:GLN:H	2.13	0.52
1:B:666:THR:HA	1:B:706:ASN:HB2	1.92	0.52
1:A:372:THR:CG2	1:A:400:GLU:HG3	2.39	0.52
1:A:747:GLN:O	1:A:751:ILE:HG13	2.09	0.52
1:A:80:THR:CG2	1:A:81:ILE:N	2.72	0.52
1:B:291:LEU:CD1	1:B:296:ILE:HG22	2.40	0.52
1:B:115:ILE:HG21	1:B:138:THR:HG23	1.91	0.52
1:B:252:GLN:NE2	3:B:841:HOH:O	2.43	0.51
1:A:466:LYS:O	1:A:467:GLY:O	2.27	0.51
1:A:4:ASN:ND2	1:A:5:GLU:H	2.08	0.51
1:A:332:ILE:CG2	1:A:368:GLU:HG3	2.40	0.51
1:B:401:ASN:ND2	1:B:404:LEU:HB2	2.24	0.51
1:A:360:LEU:HD12	1:A:365:PRO:HA	1.92	0.51
1:A:624:ARG:HH11	1:A:624:ARG:CG	2.23	0.51
1:B:752:THR:O	1:B:752:THR:HG22	2.09	0.51
1:A:115:ILE:HG22	3:A:1006:HOH:O	2.08	0.51
1:A:215:GLN:H	1:A:215:GLN:CD	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:NZ	1:A:194:LYS:HB3	2.26	0.51
1:A:80:THR:HG22	1:A:82:THR:N	2.23	0.51
1:B:80:THR:CG2	1:B:81:ILE:N	2.73	0.51
1:B:476:MET:O	1:B:477:GLU:C	2.48	0.51
1:A:752:THR:O	1:A:752:THR:HG22	2.10	0.51
1:B:344:ASP:OD1	1:B:346:ARG:HG2	2.10	0.51
1:B:322:GLU:CD	3:B:900:HOH:O	2.48	0.51
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.76	0.51
1:A:132:MET:HE1	1:A:135:LYS:HD3	1.92	0.51
1:A:40:GLU:CD	1:A:40:GLU:H	2.14	0.51
1:B:433:GLY:O	1:B:434:ALA:O	2.28	0.51
1:B:119:GLU:HG2	1:B:129:LEU:HD12	1.93	0.51
1:A:302:GLN:HG2	3:A:899:HOH:O	2.10	0.50
1:B:624:ARG:CG	1:B:624:ARG:HH11	2.25	0.50
1:A:526:ILE:HD11	1:A:584:PHE:CD2	2.46	0.50
1:A:386:PHE:O	1:A:390:VAL:HG23	2.12	0.50
1:A:605:THR:O	1:A:608:SER:HB2	2.12	0.50
1:B:545:LYS:O	1:B:557:PHE:HA	2.12	0.49
1:B:637:HIS:H	1:B:637:HIS:CD2	2.30	0.49
1:A:677:ASP:CG	1:A:680:VAL:HG23	2.33	0.49
1:B:600:THR:HG22	1:B:601:GLN:N	2.27	0.49
1:B:398:GLN:HB3	1:B:731:ARG:NH1	2.27	0.49
1:A:291:LEU:CD1	1:A:296:ILE:HG22	2.41	0.49
1:A:97:VAL:HG12	1:A:240:TYR:CE2	2.48	0.49
1:A:10:ALA:O	1:A:289:ARG:NH2	2.41	0.49
1:B:199:GLN:HG2	1:B:516:ARG:HB2	1.93	0.49
1:B:40:GLU:HB3	1:B:43:LEU:HD12	1.95	0.49
1:B:360:LEU:HD12	1:B:365:PRO:HA	1.94	0.49
1:A:398:GLN:HB3	1:A:731:ARG:NH1	2.27	0.49
1:B:97:VAL:HG12	1:B:240:TYR:CE2	2.48	0.49
1:B:186:LEU:HD13	1:B:187:TYR:CZ	2.48	0.49
1:B:312:LEU:CB	1:B:369:PRO:HG3	2.43	0.48
1:B:132:MET:O	1:B:132:MET:HE3	2.13	0.48
1:A:119:GLU:HG2	1:A:129:LEU:HD12	1.95	0.48
1:A:470:LEU:HD13	1:A:546:PRO:CG	2.42	0.48
1:A:600:THR:HG22	1:A:601:GLN:N	2.29	0.48
1:B:540:LYS:O	1:B:540:LYS:HG2	2.12	0.48
1:B:92:GLN:NE2	1:B:92:GLN:N	2.58	0.48
1:A:368:GLU:HA	1:A:369:PRO:C	2.33	0.48
1:B:291:LEU:HD12	1:B:296:ILE:O	2.14	0.48
1:A:350:THR:O	1:A:353:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:HIS:CD2	1:A:637:HIS:H	2.29	0.48
1:A:388:ALA:O	1:A:392:ILE:HG13	2.13	0.48
1:B:637:HIS:HE1	1:B:749:ASP:OD1	1.96	0.48
1:B:743:THR:OG1	1:B:746:GLN:HG3	2.13	0.48
1:A:302:GLN:OE1	1:A:355:ARG:HA	2.14	0.48
1:B:328:SER:HB3	1:B:746:GLN:NE2	2.29	0.48
1:A:641:GLN:HG2	3:A:969:HOH:O	2.12	0.48
1:B:388:ALA:O	1:B:392:ILE:HG13	2.13	0.48
1:A:637:HIS:HE1	1:A:749:ASP:OD1	1.97	0.48
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.79	0.48
1:A:401:ASN:ND2	1:A:404:LEU:HB2	2.29	0.48
1:A:97:VAL:HG12	1:A:98:GLY:N	2.29	0.48
1:A:92:GLN:HE21	1:A:92:GLN:H	1.58	0.47
1:B:677:ASP:CG	1:B:680:VAL:HG23	2.34	0.47
1:A:291:LEU:HD12	1:A:296:ILE:O	2.14	0.47
1:B:467:GLY:O	1:B:548:ARG:NH2	2.48	0.47
1:A:486:LEU:HD12	1:A:584:PHE:CE1	2.49	0.47
1:B:486:LEU:HD12	1:B:584:PHE:CE1	2.50	0.47
1:A:302:GLN:CG	3:A:899:HOH:O	2.63	0.47
1:B:97:VAL:HG12	1:B:98:GLY:N	2.29	0.47
1:B:302:GLN:OE1	1:B:355:ARG:HA	2.15	0.47
1:B:165:LEU:HA	1:B:165:LEU:HD23	1.78	0.47
1:B:332:ILE:HG23	1:B:368:GLU:HG3	1.97	0.47
1:A:151:VAL:HB	1:A:496:ILE:HD13	1.95	0.47
1:A:199:GLN:HG2	1:A:516:ARG:HB2	1.97	0.47
1:B:704:HIS:CG	1:B:705:LEU:N	2.83	0.46
1:A:132:MET:HE3	1:A:132:MET:O	2.15	0.46
1:B:302:GLN:HG2	3:B:967:HOH:O	2.14	0.46
1:A:743:THR:OG1	1:A:746:GLN:HG3	2.15	0.46
1:A:186:LEU:HD13	1:A:187:TYR:CZ	2.50	0.46
1:A:333:TRP:HE1	1:A:735:TYR:HB3	1.80	0.46
1:B:159:CYS:HB3	1:B:165:LEU:HB2	1.97	0.46
1:B:357:LEU:HA	1:B:371:MET:HE3	1.96	0.46
1:B:333:TRP:HE1	1:B:735:TYR:HB3	1.80	0.46
1:B:176:ARG:HD2	1:B:430:GLN:NE2	2.31	0.46
1:B:270:ASN:HA	1:B:270:ASN:HD22	1.53	0.46
1:B:372:THR:HG21	1:B:400:GLU:HG3	1.98	0.46
1:B:409:PHE:CE2	1:B:422:PRO:HB2	2.50	0.46
1:A:409:PHE:CE2	1:A:422:PRO:HB2	2.49	0.46
1:B:88:TYR:CE2	1:B:97:VAL:HG11	2.51	0.46
1:B:80:THR:HG22	1:B:82:THR:N	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:VAL:CG2	1:A:662:GLY:HA3	2.46	0.45
1:A:153:THR:CG2	1:B:204:GLN:HG3	2.46	0.45
1:A:312:LEU:CB	1:A:369:PRO:HG3	2.47	0.45
1:A:148:VAL:HA	1:A:496:ILE:HD11	1.97	0.45
1:A:603:VAL:HG11	1:A:633:ALA:HB2	1.98	0.45
1:B:600:THR:CG2	1:B:601:GLN:N	2.79	0.45
1:B:386:PHE:O	1:B:390:VAL:HG23	2.17	0.45
1:A:332:ILE:HG23	1:A:368:GLU:OE2	2.16	0.45
1:A:40:GLU:HB3	1:A:43:LEU:HD12	1.98	0.45
1:B:677:ASP:O	1:B:681:ARG:HG3	2.16	0.45
1:B:578:VAL:HG13	1:B:655:PRO:HD3	1.98	0.45
1:A:97:VAL:HG12	1:A:240:TYR:CD2	2.52	0.45
1:A:270:ASN:HA	1:A:270:ASN:HD22	1.53	0.45
1:B:368:GLU:HA	1:B:369:PRO:C	2.35	0.45
1:B:602:SER:HB3	1:B:661:ASP:CB	2.28	0.45
1:A:401:ASN:HB2	1:A:693:PHE:CD1	2.52	0.45
1:A:367:PRO:HG2	1:A:738:ARG:HG3	1.99	0.45
1:B:420:VAL:O	1:B:422:PRO:HD3	2.16	0.45
1:B:453:LYS:HB3	1:B:454:LEU:HD22	1.98	0.45
1:A:332:ILE:HG21	3:A:791:HOH:O	2.16	0.45
1:B:127:ARG:NH1	1:B:127:ARG:HG3	2.31	0.45
1:A:182:ARG:NH2	1:A:425:VAL:CG2	2.74	0.45
1:A:81:ILE:HG13	3:A:963:HOH:O	2.17	0.45
1:B:151:VAL:HG12	1:B:151:VAL:O	2.16	0.45
1:B:637:HIS:CE1	1:B:749:ASP:OD1	2.70	0.45
1:B:367:PRO:HG2	1:B:738:ARG:HG3	1.99	0.45
1:B:431:PHE:HB3	1:B:498:HIS:CD2	2.51	0.45
1:B:569:ASN:O	1:B:571:PRO:HD3	2.17	0.45
1:A:359:THR:CA	1:A:362:THR:HG22	2.37	0.45
1:A:704:HIS:CG	1:A:705:LEU:N	2.85	0.45
1:A:302:GLN:CD	1:A:358:ASN:HD22	2.20	0.45
1:B:332:ILE:HG23	1:B:368:GLU:CG	2.47	0.44
1:B:706:ASN:HB3	1:B:731:ARG:HB3	1.99	0.44
1:A:603:VAL:CG1	1:A:633:ALA:HB2	2.46	0.44
1:B:60:GLY:O	1:B:64:GLU:HG3	2.17	0.44
1:B:445:ALA:HA	1:B:482:PHE:CE1	2.53	0.44
1:B:603:VAL:HG11	1:B:633:ALA:HB2	2.00	0.44
1:B:309:VAL:HG21	1:B:359:THR:HG21	2.00	0.44
1:B:420:VAL:CG2	1:B:662:GLY:HA3	2.47	0.44
1:B:79:SER:HB3	1:B:110:ILE:HD13	1.99	0.44
1:B:545:LYS:HD2	1:B:558:GLU:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ASN:HD21	1:B:734:GLY:CA	2.30	0.44
1:A:372:THR:HG21	1:A:400:GLU:HG3	2.00	0.44
1:A:344:ASP:OD2	1:A:346:ARG:HD3	2.18	0.44
1:B:101:THR:OG1	1:B:102:GLU:N	2.51	0.44
1:B:97:VAL:HG12	1:B:240:TYR:CD2	2.52	0.44
1:B:302:GLN:CD	1:B:358:ASN:HD22	2.20	0.44
1:A:420:VAL:O	1:A:422:PRO:HD3	2.18	0.44
1:B:329:GLY:HA3	1:B:737:VAL:HG22	1.99	0.44
1:B:357:LEU:HD12	1:B:357:LEU:N	2.31	0.44
1:A:547:ILE:HD11	1:A:558:GLU:HG3	1.99	0.43
1:A:88:TYR:CE2	1:A:97:VAL:HG11	2.52	0.43
1:B:367:PRO:HA	1:B:736:ALA:HB3	2.00	0.43
1:A:33:TYR:CE2	1:A:35:PRO:HG3	2.53	0.43
1:A:600:THR:CG2	1:A:601:GLN:N	2.81	0.43
1:B:442:MET:HA	1:B:479:MET:CE	2.48	0.43
1:A:270:ASN:O	1:A:271:GLY:C	2.57	0.43
1:B:507:GLU:HB3	1:B:510:LEU:HD13	2.00	0.43
1:B:332:ILE:HG23	1:B:368:GLU:OE2	2.18	0.43
1:A:233:MET:HE1	1:A:261:GLY:HA2	1.98	0.43
1:B:350:THR:O	1:B:353:SER:HB2	2.18	0.43
1:B:182:ARG:NH2	1:B:425:VAL:CG2	2.76	0.43
1:A:4:ASN:CG	1:A:5:GLU:H	2.22	0.43
1:B:148:VAL:HA	1:B:496:ILE:HD11	2.00	0.43
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.33	0.43
1:A:465:ILE:CD1	1:A:475:VAL:HG22	2.49	0.43
1:B:101:THR:CG2	1:B:106:LYS:HB3	2.41	0.43
1:A:637:HIS:CE1	1:A:749:ASP:OD1	2.71	0.43
1:B:603:VAL:CG1	1:B:633:ALA:HB2	2.49	0.43
1:B:233:MET:HE3	1:B:261:GLY:HA2	1.99	0.43
1:B:401:ASN:HB2	1:B:693:PHE:CD1	2.53	0.43
1:A:540:LYS:O	1:A:540:LYS:HG2	2.18	0.43
1:B:556:ASP:C	1:B:557:PHE:CD1	2.92	0.43
1:A:547:ILE:HD11	1:A:558:GLU:CG	2.48	0.43
1:A:706:ASN:HD21	1:A:734:GLY:CA	2.32	0.43
1:A:357:LEU:HA	1:A:371:MET:HE3	2.01	0.43
1:A:6:LYS:NZ	1:A:247:PRO:O	2.52	0.43
1:B:151:VAL:HB	1:B:496:ILE:HD13	2.00	0.43
1:B:628:PRO:HG3	3:B:826:HOH:O	2.19	0.43
1:B:571:PRO:O	1:B:575:ASP:HB2	2.19	0.43
1:A:251:ALA:HA	1:A:286:TYR:HB3	2.01	0.43
1:B:196:LYS:HA	1:B:196:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:THR:CA	1:B:362:THR:HG22	2.38	0.42
1:A:332:ILE:HG23	1:A:368:GLU:HG3	2.01	0.42
1:A:86:ALA:HA	1:A:240:TYR:CZ	2.54	0.42
1:A:60:GLY:O	1:A:64:GLU:HG3	2.19	0.42
1:B:669:ILE:O	1:B:709:VAL:HA	2.19	0.42
1:B:364:GLY:HA3	1:B:727:GLN:NE2	2.32	0.42
1:A:329:GLY:HA3	1:A:737:VAL:HG22	2.02	0.42
1:A:79:SER:HB3	1:A:110:ILE:HD13	2.02	0.42
1:A:6:LYS:O	1:A:7:LEU:C	2.58	0.42
1:A:151:VAL:HG12	1:A:151:VAL:O	2.18	0.42
1:A:330:ASP:N	1:A:331:PRO:CD	2.82	0.42
1:B:251:ALA:HA	1:B:286:TYR:HB3	2.02	0.42
1:B:162:SER:OG	1:B:164:VAL:HG12	2.19	0.42
1:A:101:THR:OG1	1:A:102:GLU:N	2.52	0.42
1:B:86:ALA:HA	1:B:240:TYR:CZ	2.54	0.42
1:B:438:LEU:HA	1:B:438:LEU:HD23	1.82	0.42
1:B:233:MET:HE1	1:B:261:GLY:HA2	1.98	0.42
1:A:710:MET:HE2	1:A:710:MET:HB3	1.93	0.42
1:B:302:GLN:CG	3:B:967:HOH:O	2.67	0.42
1:A:510:LEU:HD12	1:A:510:LEU:N	2.35	0.42
1:A:4:ASN:HD22	1:A:6:LYS:N	2.07	0.42
1:B:160:ARG:HA	1:B:165:LEU:O	2.19	0.42
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.84	0.42
1:B:543:LYS:CB	1:B:560:GLU:HB3	2.43	0.42
1:A:357:LEU:N	1:A:357:LEU:HD12	2.35	0.42
1:B:549:ASP:O	1:B:551:ASP:N	2.52	0.42
1:A:526:ILE:HD11	1:A:584:PHE:CE2	2.55	0.42
1:B:270:ASN:O	1:B:271:GLY:C	2.58	0.42
1:B:79:SER:HB2	1:B:108:ALA:HB1	2.02	0.41
1:A:19:TRP:HD1	1:A:27:ASP:OD2	2.03	0.41
1:B:332:ILE:HD12	1:B:332:ILE:O	2.20	0.41
1:A:165:LEU:HD11	1:A:490:TYR:HA	2.01	0.41
1:B:706:ASN:OD1	1:B:731:ARG:HD3	2.21	0.41
1:A:233:MET:HE3	1:A:261:GLY:HA2	1.99	0.41
1:B:330:ASP:N	1:B:331:PRO:CD	2.83	0.41
1:A:332:ILE:HG23	1:A:368:GLU:CG	2.50	0.41
1:A:367:PRO:HA	1:A:736:ALA:HB3	2.02	0.41
1:B:510:LEU:N	1:B:510:LEU:HD12	2.35	0.41
1:A:364:GLY:HA3	1:A:727:GLN:NE2	2.30	0.41
1:B:706:ASN:HD21	1:B:734:GLY:HA2	1.85	0.41
1:A:309:VAL:HG21	1:A:359:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLU:HB3	1:A:510:LEU:HD13	2.03	0.41
1:B:348:LEU:HD13	1:B:348:LEU:HA	1.95	0.41
1:A:181:TYR:O	1:A:184:VAL:HG13	2.21	0.41
1:B:526:ILE:HA	1:B:526:ILE:HD13	1.84	0.41
1:A:79:SER:HB2	1:A:108:ALA:HB1	2.02	0.41
1:B:19:TRP:HD1	1:B:27:ASP:OD2	2.03	0.41
1:A:706:ASN:HB3	1:A:731:ARG:HB3	2.03	0.41
1:A:148:VAL:HA	1:A:496:ILE:CD1	2.50	0.41
1:B:148:VAL:HA	1:B:496:ILE:CD1	2.51	0.41
1:B:441:THR:HG22	1:B:479:MET:CE	2.51	0.41
1:A:446:ILE:HG12	1:A:465:ILE:HD12	2.02	0.41
1:B:623:ARG:NH1	1:B:627:ALA:O	2.54	0.41
1:B:182:ARG:HH22	1:B:425:VAL:CG2	2.31	0.41
1:B:568:ASN:O	1:B:642:LYS:HD2	2.20	0.41
1:A:677:ASP:O	1:A:681:ARG:HG3	2.21	0.40
1:A:332:ILE:O	1:A:333:TRP:HB2	2.20	0.40
1:A:710:MET:CE	1:A:730:ILE:HG22	2.50	0.40
1:B:438:LEU:HG	1:B:526:ILE:HD12	2.03	0.40
1:A:545:LYS:O	1:A:545:LYS:HG3	2.20	0.40
1:B:295:LYS:O	1:B:296:ILE:HD12	2.22	0.40
1:A:752:THR:O	1:A:752:THR:CG2	2.69	0.40
1:A:271:GLY:HA3	1:A:274:MET:SD	2.61	0.40
1:B:33:TYR:CE2	1:B:35:PRO:HG3	2.56	0.40
1:A:565:GLN:NE2	1:A:639:ARG:HD3	2.36	0.40
1:B:362:THR:CG2	1:B:363:MET:HG3	2.34	0.40
1:A:481:HIS:O	1:A:484:ASP:HB2	2.21	0.40
1:A:338:ILE:HG22	1:A:339:GLY:N	2.36	0.40
1:B:711:ASN:HB3	1:B:713:GLU:OE1	2.22	0.40
1:A:97:VAL:CG1	1:A:240:TYR:CD2	3.04	0.40
1:B:394:THR:O	1:B:395:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	757/759 (100%)	706 (93%)	44 (6%)	7 (1%)	21	42
1	B	757/759 (100%)	703 (93%)	46 (6%)	8 (1%)	17	36
All	All	1514/1518 (100%)	1409 (93%)	90 (6%)	15 (1%)	19	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	ALA
1	B	434	ALA
1	B	550	GLU
1	A	271	GLY
1	A	467	GLY
1	A	606	ILE
1	A	733	SER
1	B	271	GLY
1	B	452	GLU
1	B	606	ILE
1	B	733	SER
1	B	723	GLU
1	A	723	GLU
1	A	4	ASN
1	B	169	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	638/638 (100%)	597 (94%)	41 (6%)	22	43
1	B	638/638 (100%)	598 (94%)	40 (6%)	22	44
All	All	1276/1276 (100%)	1195 (94%)	81 (6%)	22	44

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	40	GLU
1	A	75	THR
1	A	80	THR
1	A	92	GLN
1	A	129	LEU
1	A	152	TYR
1	A	157	LEU
1	A	165	LEU
1	A	184	VAL
1	A	186	LEU
1	A	257	TRP
1	A	260	PHE
1	A	270	ASN
1	A	278	ARG
1	A	291	LEU
1	A	292	LYS
1	A	296	ILE
1	A	318	LEU
1	A	326	LEU
1	A	332	ILE
1	A	346	ARG
1	A	348	LEU
1	A	360	LEU
1	A	371	MET
1	A	400	GLU
1	A	430	GLN
1	A	431	PHE
1	A	435	ARG
1	A	438	LEU
1	A	470	LEU
1	A	490	TYR
1	A	496	ILE
1	A	513	LEU
1	A	529	LEU
1	A	531	VAL
1	A	543	LYS
1	A	595	ARG
1	A	624	ARG
1	A	660	LYS
1	A	733	SER
1	B	5	GLU
1	B	40	GLU

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Mol	Chain	Res	Type
1	B	75	THR
1	B	80	THR
1	B	92	GLN
1	B	129	LEU
1	B	152	TYR
1	B	157	LEU
1	B	184	VAL
1	B	186	LEU
1	B	257	TRP
1	B	260	PHE
1	B	270	ASN
1	B	278	ARG
1	B	291	LEU
1	B	292	LYS
1	B	296	ILE
1	B	318	LEU
1	B	326	LEU
1	B	332	ILE
1	B	346	ARG
1	B	348	LEU
1	B	360	LEU
1	B	362	THR
1	B	371	MET
1	B	400	GLU
1	B	431	PHE
1	B	435	ARG
1	B	438	LEU
1	B	468	ASP
1	B	479	MET
1	B	490	TYR
1	B	496	ILE
1	B	513	LEU
1	B	529	LEU
1	B	531	VAL
1	B	543	LYS
1	B	595	ARG
1	B	624	ARG
1	B	660	LYS

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	4	ASN
1	A	92	GLN
1	A	270	ASN
1	A	358	ASN
1	A	430	GLN
1	A	565	GLN
1	A	637	HIS
1	A	684	ASN
1	A	711	ASN
1	B	92	GLN
1	B	144	HIS
1	B	270	ASN
1	B	358	ASN
1	B	430	GLN
1	B	637	HIS
1	B	684	ASN
1	B	711	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
2	OXM	A	761	-	2,5,5	0.30	0	2,6,6	0.87	0
2	OXM	B	762	-	2,5,5	0.09	0	2,6,6	1.11	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
2	OXM	A	761	-	-	0/0/4/4	0/0/0/0
2	OXM	B	762	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 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	759/759 (100%)	-0.14	14 (1%) 71 66	27, 45, 65, 100	0
1	B	759/759 (100%)	-0.03	26 (3%) 49 41	30, 48, 73, 96	0
All	All	1518/1518 (100%)	-0.09	40 (2%) 59 53	27, 47, 70, 100	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLU	7.8
1	A	1	SER	7.6
1	B	1	SER	6.6
1	B	2	GLU	4.5
1	B	419	CYS	4.0
1	A	3	LEU	3.5
1	B	273	ALA	3.5
1	A	419	CYS	3.4
1	B	467	GLY	2.9
1	B	333	TRP	2.8
1	B	420	VAL	2.8
1	A	676	LYS	2.7
1	A	418	CYS	2.7
1	B	418	CYS	2.7
1	A	334	ALA	2.7
1	B	560	GLU	2.7
1	B	5	GLU	2.6
1	B	3	LEU	2.5
1	A	550	GLU	2.5
1	A	333	TRP	2.4
1	B	541	TYR	2.4
1	B	421	SER	2.4
1	B	416	ILE	2.4
1	B	733	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	559	ILE	2.3
1	B	664	SER	2.3
1	B	734	GLY	2.2
1	A	721	ASN	2.2
1	B	561	GLY	2.2
1	A	275	SER	2.1
1	B	468	ASP	2.1
1	A	335	THR	2.1
1	B	270	ASN	2.1
1	B	335	THR	2.1
1	B	434	ALA	2.1
1	A	680	VAL	2.0
1	A	332	ILE	2.0
1	B	275	SER	2.0
1	B	272	ALA	2.0
1	B	417	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	OXM	A	761	6/6	0.95	0.35	2.46	41,43,44,45	0
2	OXM	B	762	6/6	0.98	0.29	-0.28	42,43,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.