Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 10:28 AM EDT

PDB ID	:	3H3O
Title	:	Glycerol Kinase H232R with Ethylene Glycol
Authors	:	Yeh, J.I.; Kettering, R.D.
Deposited on	:	2009-04-16
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

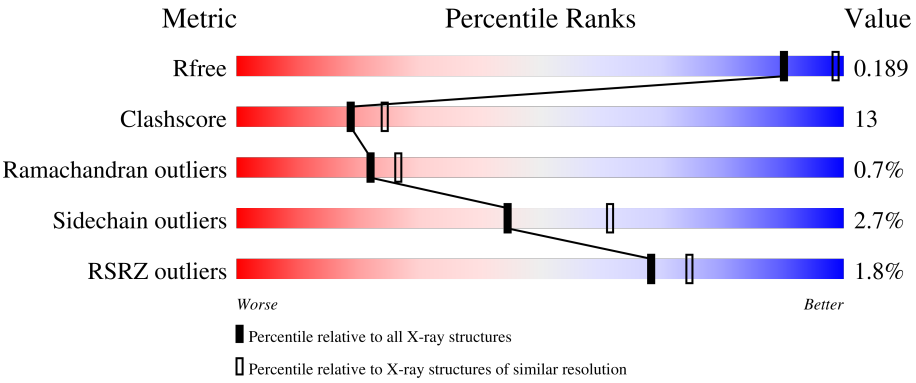
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	B	506	73% 24%
1	C	506	3% 65% 32%
1	O	506	75% 22%
1	X	506	2% 74% 24%

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	EDO	X	3133	-	-	X	-
3	PO4	X	508	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15718 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.

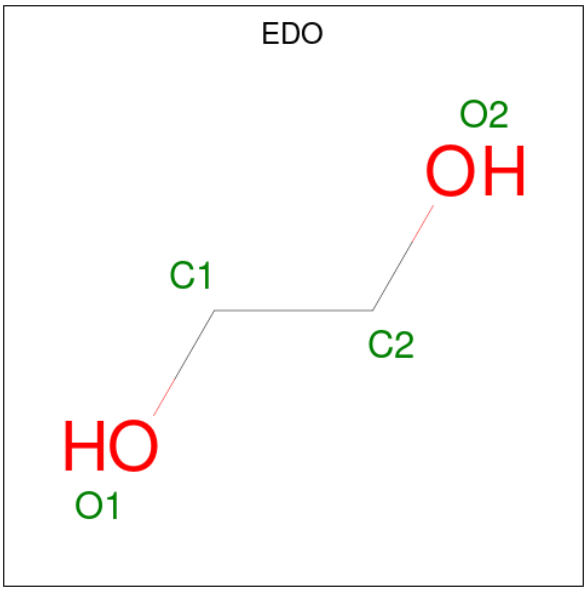
- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3863	2448	645	756	14			
1	X	499	Total	C	N	O	S	0	0	0
			3864	2448	645	757	14			
1	B	499	Total	C	N	O	S	0	0	0
			3857	2443	644	756	14			
1	C	498	Total	C	N	O	S	0	0	0
			3859	2445	644	756	14			

There are 4 discrepancies between the modelled and reference sequences:

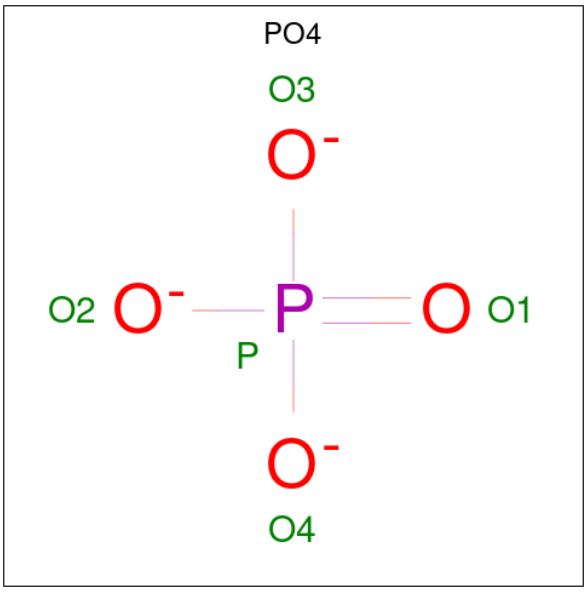
Chain	Residue	Modelled	Actual	Comment	Reference
O	232	ARG	HIS	engineered mutation	UNP O34153
X	232	ARG	HIS	engineered mutation	UNP O34153
B	232	ARG	HIS	engineered mutation	UNP O34153
C	232	ARG	HIS	engineered mutation	UNP O34153

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total O P 5 4 1	0	0
3	O	1	Total O P 5 4 1	0	0
3	O	1	Total O P 5 4 1	0	0
3	X	1	Total O P 5 4 1	0	0
3	X	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

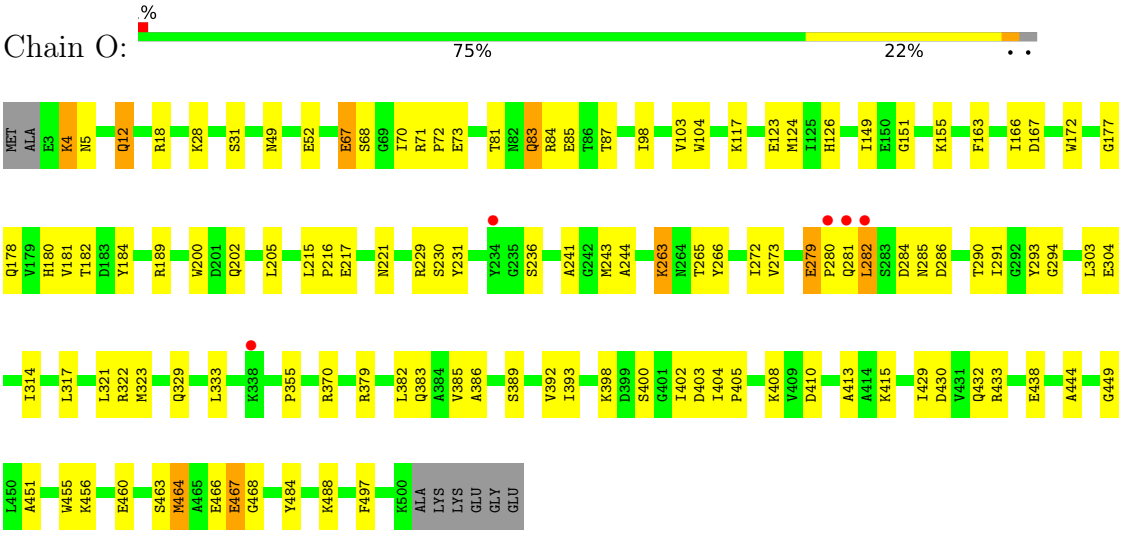
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	57	Total O 57 57	0	0
4	X	66	Total O 66 66	0	0
4	B	47	Total O 47 47	0	0
4	C	30	Total O 30 30	0	0

3 Residue-property plots (i)

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

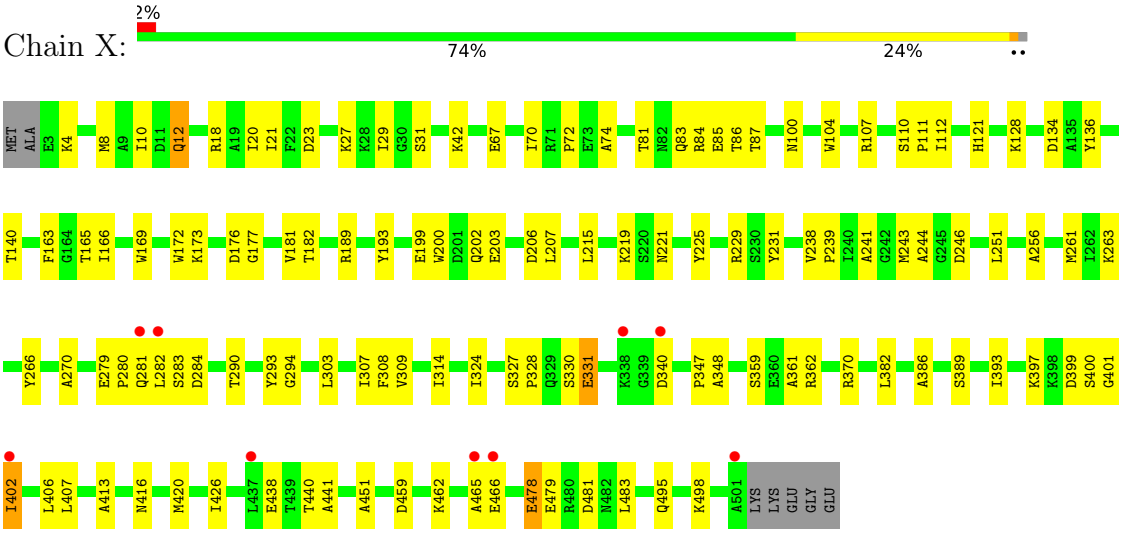
• Molecule 1: Glycerol kinase

Chain O:



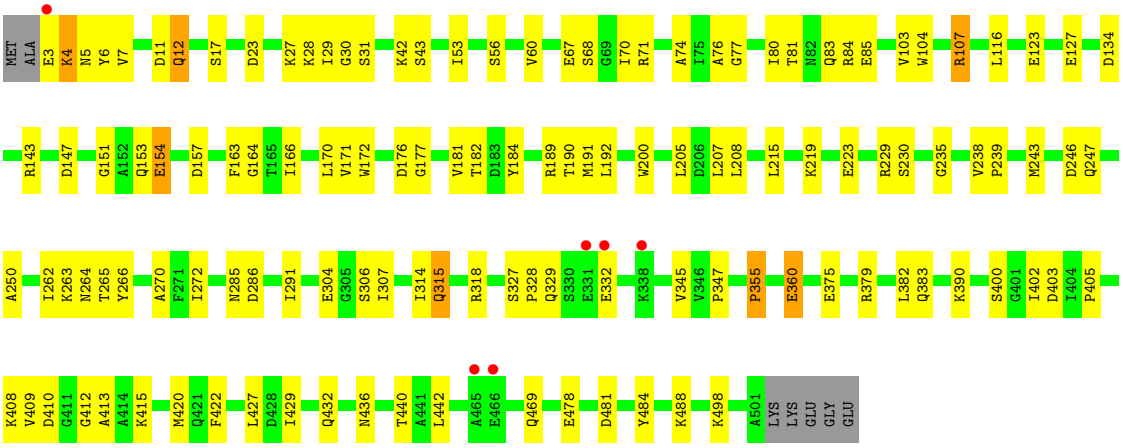
• Molecule 1: Glycerol kinase

Chain X:



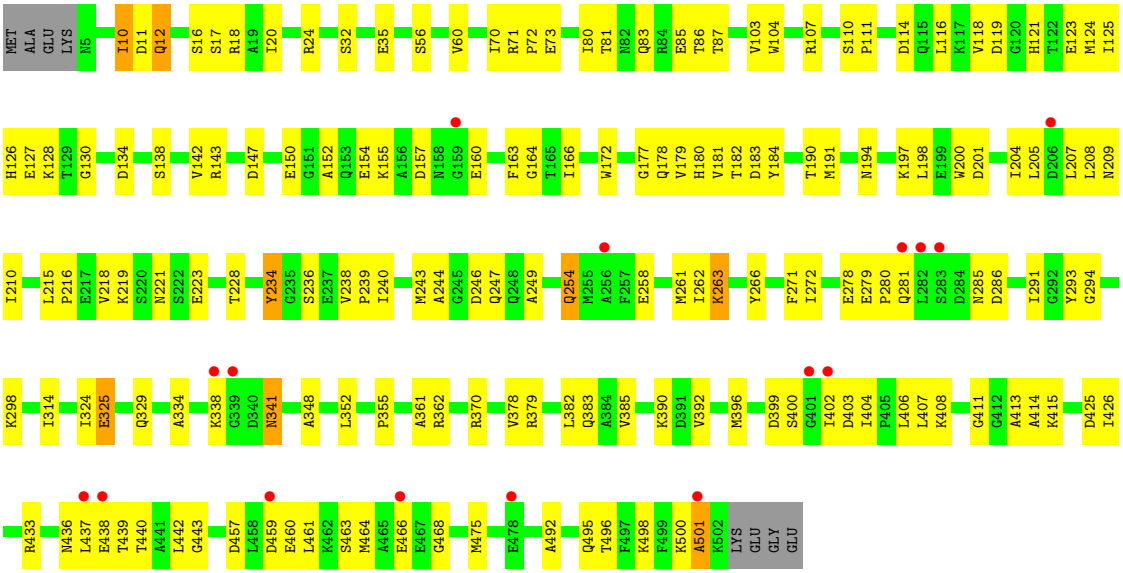
• Molecule 1: Glycerol kinase

Chain B:



• Molecule 1: Glycerol kinase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.84Å 104.28Å 114.24Å 90.00° 114.13° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 49.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 81.8 (49.45-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.206 0.179 , 0.189	Depositor DCC
R_{free} test set	3894 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15718	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PO4

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	B	0.35	0/3937	0.59	0/5340
1	C	0.32	0/3939	0.56	0/5342
1	O	0.38	0/3943	0.64	2/5346 (0.0%)
1	X	0.35	0/3944	0.60	0/5349
All	All	0.35	0/15763	0.60	2/21377 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	84	ARG	N-CA-C	7.85	132.21	111.00
1	O	83	GLN	N-CA-C	-5.14	97.11	111.00

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	B	3857	0	3739	89	0
1	C	3859	0	3752	127	0
1	O	3863	0	3760	88	0
1	X	3864	0	3754	98	0
2	B	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	6	0	0
2	O	4	0	6	0	0
2	X	20	0	30	10	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	O	15	0	0	0	0
3	X	10	0	0	2	0
4	B	47	0	0	0	0
4	C	30	0	0	0	0
4	O	57	0	0	2	0
4	X	66	0	0	0	0
All	All	15718	0	15065	401	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 13.

All (401) 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:X:221:ASN:HD22	1:X:294:GLY:H	1.06	0.96
1:O:221:ASN:HD22	1:O:294:GLY:H	1.17	0.92
1:B:12:GLN:HE22	1:B:83:GLN:HE21	1.16	0.88
1:X:331:GLU:HG2	1:X:416:ASN:ND2	1.90	0.86
1:B:219:LYS:HE2	1:B:223:GLU:OE2	1.75	0.86
1:B:85:GLU:OE2	1:B:189:ARG:HD2	1.75	0.85
1:O:400:SER:HB2	1:O:402:ILE:HD13	1.57	0.85
1:X:181:VAL:HG21	1:X:219:LYS:HD2	1.60	0.83
1:C:201:ASP:O	1:C:205:LEU:HD23	1.79	0.82
1:X:221:ASN:ND2	1:X:294:GLY:H	1.76	0.82
1:O:71:ARG:HD3	1:X:231:TYR:HB2	1.62	0.81
1:O:12:GLN:HE22	1:O:83:GLN:HE21	1.28	0.80
1:C:221:ASN:HD22	1:C:294:GLY:H	1.30	0.77
1:X:18:ARG:NE	1:X:20:ILE:HD11	2.00	0.76
1:X:176:ASP:HB3	1:X:229:ARG:NH1	2.03	0.74
1:C:254:GLN:NE2	1:C:408:LYS:HB3	2.01	0.74
1:O:415:LYS:HD3	1:O:415:LYS:C	2.07	0.73
1:C:254:GLN:HE22	1:C:408:LYS:HB3	1.54	0.73
1:C:143:ARG:NH1	1:C:209:ASN:HB3	2.04	0.72
1:O:85:GLU:OE2	1:O:189:ARG:HD2	1.90	0.72
1:C:402:ILE:HG22	1:C:403:ASP:H	1.55	0.72
1:O:81:THR:HG23	1:O:444:ALA:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:ILE:HD13	1:X:70:ILE:HD11	1.72	0.71
1:X:193:TYR:HE1	2:X:3132:EDO:H22	1.55	0.71
1:X:308:PHE:HB2	2:X:3133:EDO:H12	1.73	0.71
1:C:114:ASP:O	1:C:118:VAL:HG23	1.90	0.70
1:X:18:ARG:CZ	1:X:20:ILE:HD11	2.22	0.70
1:C:155:LYS:O	1:C:160:GLU:HB3	1.92	0.69
1:B:250:ALA:HB3	1:B:263:LYS:HE2	1.73	0.69
1:C:12:GLN:HE22	1:C:83:GLN:HE21	1.41	0.69
1:O:279:GLU:OE1	1:O:281:GLN:HB3	1.93	0.68
1:C:266:TYR:HB3	1:C:413:ALA:HB3	1.74	0.68
1:X:199:GLU:HA	2:X:3132:EDO:H21	1.74	0.68
1:O:68:SER:HB2	1:O:70:ILE:HD13	1.74	0.68
1:X:495:GLN:O	1:X:498:LYS:HE2	1.94	0.68
1:C:150:GLU:CD	1:C:150:GLU:H	1.97	0.67
1:X:279:GLU:HB3	1:X:281:GLN:HG2	1.77	0.67
1:B:379:ARG:O	1:B:383:GLN:HG3	1.95	0.67
1:C:402:ILE:HG22	1:C:403:ASP:N	2.10	0.66
1:B:12:GLN:NE2	1:B:83:GLN:HE21	1.90	0.65
1:B:176:ASP:HB3	1:B:229:ARG:NH1	2.12	0.65
1:X:266:TYR:HB3	1:X:413:ALA:HB3	1.77	0.64
1:X:314:ILE:HD11	1:X:382:LEU:CD2	2.27	0.63
1:B:23:ASP:OD2	1:B:27:LYS:HB3	1.98	0.63
1:O:221:ASN:ND2	1:O:294:GLY:H	1.92	0.63
1:O:4:LYS:O	1:O:5:ASN:HB2	1.99	0.63
1:X:165:THR:HG22	1:X:166:ILE:H	1.60	0.63
1:C:324:ILE:HG23	1:C:329:GLN:HE21	1.63	0.63
1:O:379:ARG:O	1:O:383:GLN:HG3	1.99	0.62
1:O:151:GLY:O	1:O:155:LYS:HG3	1.98	0.62
1:B:28:LYS:HE2	1:B:31:SER:HB2	1.82	0.62
1:O:466:GLU:O	1:O:467:GLU:HB3	2.00	0.62
1:C:128:LYS:O	1:C:194:ASN:HA	2.00	0.62
1:X:324:ILE:HD11	1:X:330:SER:N	2.15	0.61
1:C:10:ILE:HD13	1:C:10:ILE:C	2.21	0.61
1:B:12:GLN:HE21	1:B:166:ILE:HG21	1.65	0.61
1:C:24:ARG:O	1:C:464:MET:HE1	2.01	0.61
1:C:87:THR:HG23	1:C:163:PHE:CE1	2.36	0.61
1:X:459:ASP:HA	1:X:462:LYS:HE2	1.83	0.60
1:B:11:ASP:HA	1:B:81:THR:HG23	1.83	0.60
1:C:460:GLU:O	1:C:463:SER:HB3	1.99	0.60
1:X:308:PHE:HB2	2:X:3133:EDO:C1	2.32	0.60
1:C:83:GLN:HG3	1:C:83:GLN:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:HD12	1:B:208:LEU:HG	1.83	0.60
1:C:325:GLU:H	1:C:329:GLN:NE2	1.99	0.60
1:O:81:THR:CG2	1:O:444:ALA:HB2	2.32	0.60
1:C:258:GLU:HB3	1:C:261:MET:SD	2.42	0.60
1:C:390:LYS:HD2	1:C:426:ILE:HG22	1.82	0.60
1:O:266:TYR:HB3	1:O:413:ALA:HB3	1.82	0.59
1:C:154:GLU:HA	1:C:157:ASP:OD2	2.02	0.59
1:O:12:GLN:NE2	1:O:83:GLN:HE21	2.00	0.59
1:X:309:VAL:HG23	2:X:3133:EDO:H11	1.84	0.59
1:C:180:HIS:CE1	1:C:216:PRO:HB3	2.38	0.59
1:B:67:GLU:O	1:B:67:GLU:HG2	2.01	0.59
1:C:181:VAL:HG22	1:C:182:THR:N	2.17	0.59
1:O:71:ARG:HD2	1:O:73:GLU:CD	2.23	0.59
1:B:184:TYR:HB3	1:B:291:ILE:HG21	1.85	0.59
1:X:181:VAL:CG2	1:X:219:LYS:HD2	2.33	0.59
1:B:205:LEU:HD11	1:B:215:LEU:HD11	1.85	0.59
1:C:110:SER:N	1:C:111:PRO:HD2	2.17	0.58
1:O:263:LYS:HD2	1:O:263:LYS:C	2.24	0.58
1:O:329:GLN:HG2	1:O:333:LEU:CD2	2.34	0.58
1:X:85:GLU:OE2	1:X:189:ARG:HB3	2.03	0.58
1:O:4:LYS:O	1:O:5:ASN:CB	2.52	0.58
1:B:12:GLN:HE22	1:B:83:GLN:NE2	1.95	0.58
1:B:272:ILE:N	1:B:272:ILE:HD12	2.18	0.58
1:C:143:ARG:NE	1:C:147:ASP:OD1	2.31	0.58
1:C:184:TYR:HB3	1:C:291:ILE:HG21	1.85	0.57
1:O:87:THR:HG23	1:O:163:PHE:CE1	2.38	0.57
1:C:238:VAL:HG13	1:C:239:PRO:HD2	1.87	0.57
1:O:87:THR:HG23	1:O:163:PHE:HE1	1.68	0.57
1:O:280:PRO:O	1:O:282:LEU:HD22	2.04	0.57
1:O:314:ILE:HD11	1:O:382:LEU:HD23	1.87	0.57
1:C:324:ILE:HG22	1:C:325:GLU:N	2.18	0.57
1:O:281:GLN:O	1:O:281:GLN:HG3	2.03	0.57
1:X:389:SER:O	1:X:393:ILE:HG12	2.05	0.57
1:C:83:GLN:HA	1:C:246:ASP:OD2	2.05	0.56
1:C:85:GLU:HB2	1:C:104:TRP:HB3	1.85	0.56
1:O:67:GLU:O	1:O:67:GLU:HG3	2.04	0.56
1:B:181:VAL:HG22	1:B:182:THR:N	2.21	0.56
1:X:324:ILE:CD1	1:X:330:SER:HB3	2.36	0.56
1:X:165:THR:HG22	1:X:166:ILE:N	2.20	0.56
1:C:87:THR:HG23	1:C:163:PHE:HE1	1.70	0.56
1:O:290:THR:HG22	4:O:514:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:281:GLN:O	1:X:281:GLN:HG3	2.06	0.55
1:O:189:ARG:HE	1:O:290:THR:HG21	1.71	0.55
1:C:415:LYS:HG3	1:C:437:LEU:CD1	2.36	0.55
1:X:27:LYS:O	1:X:29:ILE:HD12	2.06	0.55
1:X:189:ARG:HH11	1:X:290:THR:HG21	1.72	0.55
1:B:53:ILE:O	1:B:56:SER:HB3	2.06	0.55
1:O:178:GLN:CG	1:O:229:ARG:HH21	2.19	0.55
1:C:218:VAL:HG12	1:C:218:VAL:O	2.05	0.55
1:X:87:THR:HG23	1:X:163:PHE:HE1	1.72	0.55
1:X:20:ILE:HG12	1:X:31:SER:HB2	1.88	0.54
1:C:207:LEU:HD12	1:C:207:LEU:O	2.08	0.54
1:X:314:ILE:HD11	1:X:382:LEU:HD23	1.89	0.54
1:C:285:ASN:HB2	1:C:399:ASP:OD1	2.07	0.54
1:C:495:GLN:O	1:C:498:LYS:HE3	2.07	0.54
1:B:123:GLU:O	1:B:127:GLU:HG3	2.08	0.54
1:B:30:GLY:HA3	1:B:68:SER:HB3	1.89	0.54
1:C:205:LEU:HD13	1:C:210:ILE:HB	1.90	0.54
1:B:286:ASP:HB3	1:B:355:PRO:HB2	1.90	0.54
1:C:379:ARG:O	1:C:383:GLN:HG3	2.07	0.54
1:B:154:GLU:CD	1:B:154:GLU:H	2.11	0.54
1:X:181:VAL:HG22	1:X:182:THR:N	2.23	0.53
1:X:282:LEU:HD12	1:X:400:SER:HB3	1.90	0.53
1:C:262:ILE:HD11	1:C:272:ILE:CG2	2.39	0.53
1:X:308:PHE:HE2	3:X:508:PO4:O3	1.90	0.53
1:C:125:ILE:HG12	1:C:204:ILE:HD12	1.91	0.53
1:B:412:GLY:O	1:B:415:LYS:HG2	2.09	0.53
1:X:20:ILE:HG12	1:X:31:SER:CB	2.39	0.53
1:X:81:THR:OG1	1:X:246:ASP:HA	2.09	0.53
1:B:265:THR:HG23	1:B:410:ASP:OD1	2.09	0.53
1:B:315:GLN:HG3	1:B:318:ARG:NH2	2.23	0.53
1:B:4:LYS:CB	1:B:74:ALA:HA	2.38	0.53
1:X:324:ILE:HD12	1:X:330:SER:HB3	1.91	0.52
1:C:107:ARG:O	1:C:110:SER:HB2	2.09	0.52
1:X:406:LEU:HD12	1:X:407:LEU:H	1.74	0.52
1:C:361:ALA:O	1:C:362:ARG:NH1	2.41	0.52
1:O:189:ARG:HH22	1:O:304:GLU:CD	2.13	0.52
1:C:272:ILE:HD12	1:C:272:ILE:N	2.25	0.52
1:X:202:GLN:HE21	1:X:206:ASP:CG	2.12	0.52
1:C:200:TRP:CG	1:C:215:LEU:HD13	2.45	0.52
1:B:189:ARG:NH2	1:B:304:GLU:CD	2.63	0.52
1:B:403:ASP:O	1:B:405:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:178:GLN:HG2	1:O:229:ARG:NH2	2.24	0.52
1:C:160:GLU:HG3	1:C:160:GLU:O	2.10	0.52
1:X:200:TRP:CD2	1:X:215:LEU:HD13	2.45	0.52
1:B:266:TYR:HB3	1:B:413:ALA:HB3	1.92	0.52
1:O:230:SER:HA	1:O:236:SER:O	2.10	0.51
1:B:17:SER:O	1:B:60:VAL:HG11	2.10	0.51
1:C:12:GLN:HE21	1:C:166:ILE:HG21	1.75	0.51
1:B:28:LYS:HE2	1:B:31:SER:CB	2.40	0.51
1:C:279:GLU:OE2	1:C:279:GLU:N	2.41	0.51
1:O:314:ILE:HD11	1:O:382:LEU:CD2	2.40	0.51
1:X:241:ALA:HB1	1:X:451:ALA:HB3	1.91	0.51
1:B:154:GLU:CD	1:B:154:GLU:N	2.63	0.51
1:O:12:GLN:HE21	1:O:166:ILE:HG21	1.75	0.51
1:B:11:ASP:HA	1:B:81:THR:CG2	2.41	0.51
1:C:324:ILE:HG23	1:C:329:GLN:NE2	2.24	0.51
1:O:98:ILE:HD12	1:O:149:ILE:HG21	1.92	0.51
1:O:389:SER:O	1:O:393:ILE:HG12	2.11	0.51
1:O:438:GLU:O	1:O:438:GLU:HG3	2.10	0.51
1:O:241:ALA:HB1	1:O:451:ALA:HB3	1.93	0.51
1:O:405:PRO:O	1:O:429:ILE:HG23	2.11	0.51
1:X:400:SER:C	1:X:402:ILE:H	2.13	0.51
1:B:264:ASN:ND2	1:B:266:TYR:CZ	2.79	0.51
1:B:314:ILE:HD11	1:B:382:LEU:HD23	1.93	0.51
1:C:219:LYS:HG2	1:C:223:GLU:OE2	2.10	0.51
1:X:29:ILE:HD12	1:X:29:ILE:N	2.26	0.51
1:B:408:LYS:HA	1:B:432:GLN:O	2.12	0.50
1:B:70:ILE:HG22	1:B:71:ARG:N	2.26	0.50
1:C:403:ASP:O	1:C:404:ILE:HD13	2.12	0.50
1:C:285:ASN:O	1:C:286:ASP:HB2	2.12	0.50
1:X:8:MET:HE3	1:X:10:ILE:HD11	1.93	0.50
1:X:181:VAL:HG22	1:X:182:THR:H	1.77	0.50
1:B:484:TYR:CE2	1:B:488:LYS:HD2	2.47	0.50
1:X:314:ILE:HD11	1:X:382:LEU:HD21	1.93	0.50
1:B:250:ALA:CB	1:B:263:LYS:HE2	2.39	0.50
1:O:189:ARG:HH21	1:O:290:THR:HG21	1.77	0.50
1:B:427:LEU:HB3	1:B:429:ILE:HG12	1.94	0.50
1:O:184:TYR:HB3	1:O:291:ILE:HG21	1.92	0.49
1:X:347:PRO:O	2:X:3133:EDO:H22	2.11	0.49
1:B:285:ASN:O	1:B:286:ASP:HB2	2.12	0.49
1:C:181:VAL:CG2	1:C:182:THR:N	2.75	0.49
1:C:492:ALA:O	1:C:496:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:103:VAL:HG12	1:O:104:TRP:N	2.27	0.49
1:O:205:LEU:HD11	1:O:215:LEU:HD11	1.93	0.49
1:O:281:GLN:O	1:O:281:GLN:CG	2.60	0.49
1:O:385:VAL:HG13	1:O:386:ALA:N	2.27	0.49
1:O:433:ARG:O	1:O:468:GLY:HA3	2.11	0.49
1:X:87:THR:HG23	1:X:163:PHE:CE1	2.46	0.49
1:B:116:LEU:HD11	1:B:208:LEU:HD21	1.93	0.49
1:B:327:SER:N	1:B:328:PRO:HD2	2.27	0.49
1:C:433:ARG:HD2	1:C:437:LEU:HD21	1.93	0.49
1:C:370:ARG:HG3	1:C:370:ARG:HH11	1.75	0.49
1:O:321:LEU:O	1:O:322:ARG:HB2	2.13	0.49
1:C:406:LEU:HD12	1:C:407:LEU:H	1.76	0.49
1:X:280:PRO:O	1:X:282:LEU:HD23	2.13	0.49
1:O:167:ASP:OD2	1:O:243:MET:HE2	2.13	0.49
1:B:409:VAL:HG21	1:B:420:MET:SD	2.53	0.49
1:X:270:ALA:HB3	1:X:307:ILE:HB	1.94	0.48
1:X:438:GLU:HG3	1:X:441:ALA:HB3	1.95	0.48
1:B:80:ILE:O	1:B:243:MET:HA	2.13	0.48
1:C:178:GLN:HG2	1:C:179:VAL:HG23	1.95	0.48
1:B:436:ASN:HD21	1:B:442:LEU:HD22	1.77	0.48
1:C:18:ARG:HG3	1:C:32:SER:O	2.13	0.48
1:C:382:LEU:O	1:C:385:VAL:HG12	2.13	0.48
1:O:221:ASN:ND2	1:O:293:TYR:HA	2.28	0.48
1:C:183:ASP:OD2	1:C:243:MET:HG2	2.13	0.48
1:X:193:TYR:CE1	2:X:3132:EDO:H22	2.43	0.48
1:O:178:GLN:HG3	1:O:229:ARG:HH21	1.78	0.48
1:B:3:GLU:N	1:B:76:ALA:HA	2.28	0.48
1:B:143:ARG:NH2	1:B:147:ASP:OD1	2.45	0.48
1:O:400:SER:CB	1:O:402:ILE:HD13	2.39	0.48
1:B:345:VAL:O	1:B:347:PRO:HD3	2.14	0.48
1:X:81:THR:HG21	1:X:440:THR:HG22	1.95	0.48
1:B:176:ASP:HB3	1:B:229:ARG:HH11	1.79	0.48
1:C:143:ARG:HH12	1:C:209:ASN:HB3	1.76	0.48
1:X:107:ARG:NH2	1:X:134:ASP:OD1	2.47	0.47
1:O:28:LYS:HE3	1:O:31:SER:OG	2.14	0.47
1:O:281:GLN:O	1:O:282:LEU:HB3	2.15	0.47
1:X:386:ALA:O	1:X:426:ILE:HD11	2.15	0.47
1:B:172:TRP:CE2	1:B:177:GLY:HA2	2.49	0.47
1:O:189:ARG:NH2	1:O:304:GLU:OE1	2.47	0.47
1:B:3:GLU:O	1:B:4:LYS:CB	2.62	0.47
1:B:229:ARG:HH11	1:B:229:ARG:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:285:ASN:HD22	1:O:398:LYS:NZ	2.12	0.47
1:O:484:TYR:CE2	1:O:488:LYS:HD2	2.49	0.47
1:X:121:HIS:NE2	1:X:207:LEU:HD11	2.30	0.47
1:X:85:GLU:O	1:X:86:THR:C	2.53	0.47
1:C:119:ASP:OD2	1:C:121:HIS:NE2	2.47	0.47
1:C:325:GLU:HA	1:C:325:GLU:OE1	2.14	0.47
1:C:433:ARG:O	1:C:468:GLY:HA3	2.15	0.47
1:C:436:ASN:HD21	1:C:442:LEU:CD1	2.28	0.47
1:X:12:GLN:HE21	1:X:166:ILE:HG21	1.80	0.47
1:C:103:VAL:HG12	1:C:104:TRP:N	2.30	0.47
1:O:126:HIS:HE1	1:O:284:ASP:OD1	1.97	0.47
1:O:181:VAL:HG22	1:O:182:THR:N	2.30	0.47
1:X:256:ALA:HA	1:X:261:MET:CE	2.44	0.47
1:C:85:GLU:O	1:C:86:THR:C	2.52	0.47
1:O:71:ARG:HG2	1:O:72:PRO:HD2	1.97	0.47
1:X:85:GLU:HB2	1:X:104:TRP:HB3	1.96	0.47
1:B:84:ARG:H	2:B:1002:EDO:H22	1.80	0.47
1:B:329:GLN:O	1:B:332:GLU:HG2	2.15	0.47
1:C:314:ILE:HD11	1:C:382:LEU:HD23	1.97	0.47
1:B:200:TRP:CD2	1:B:215:LEU:HD13	2.49	0.46
1:X:110:SER:N	1:X:111:PRO:CD	2.78	0.46
1:X:172:TRP:CE2	1:X:177:GLY:HA2	2.50	0.46
1:C:249:ALA:O	1:C:443:GLY:HA3	2.16	0.46
1:X:279:GLU:C	1:X:281:GLN:H	2.19	0.46
1:C:221:ASN:HD22	1:C:294:GLY:N	2.05	0.46
1:O:180:HIS:CE1	1:O:216:PRO:HB3	2.50	0.46
1:C:172:TRP:CE2	1:C:177:GLY:HA2	2.51	0.46
1:B:192:LEU:HD22	1:B:205:LEU:HD23	1.97	0.46
1:X:221:ASN:ND2	1:X:293:TYR:HA	2.31	0.46
1:C:400:SER:HB3	1:C:402:ILE:HG13	1.97	0.46
1:X:238:VAL:HA	1:X:239:PRO:HD3	1.83	0.46
1:C:228:THR:HG22	1:C:240:ILE:HD11	1.97	0.46
1:X:241:ALA:HB1	1:X:451:ALA:CB	2.46	0.46
1:O:466:GLU:O	1:O:467:GLU:CB	2.64	0.46
1:X:21:ILE:HG21	1:X:70:ILE:HD13	1.98	0.46
1:B:6:TYR:CE1	1:B:29:ILE:HD12	2.51	0.46
1:B:107:ARG:NH2	1:B:134:ASP:OD2	2.48	0.46
1:B:400:SER:C	1:B:402:ILE:H	2.18	0.46
1:C:107:ARG:NH2	1:C:134:ASP:OD2	2.49	0.46
1:O:285:ASN:ND2	1:O:286:ASP:OD2	2.48	0.45
1:O:329:GLN:HE21	1:O:333:LEU:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:464:MET:HE2	4:O:566:HOH:O	2.16	0.45
1:X:229:ARG:HG3	1:X:229:ARG:HH11	1.81	0.45
1:C:81:THR:HG21	1:C:440:THR:HG22	1.98	0.45
1:C:180:HIS:CD2	1:C:216:PRO:HB3	2.51	0.45
1:C:263:LYS:HD2	1:C:263:LYS:C	2.37	0.45
1:O:402:ILE:HG22	1:O:403:ASP:O	2.16	0.45
1:X:29:ILE:HG22	1:X:29:ILE:O	2.16	0.45
1:B:238:VAL:HG13	1:B:239:PRO:HD2	1.98	0.45
1:C:221:ASN:ND2	1:C:293:TYR:HA	2.31	0.45
1:O:286:ASP:HB3	1:O:355:PRO:HB2	1.97	0.45
1:B:360:GLU:HB3	1:B:498:LYS:HD2	1.99	0.45
1:C:180:HIS:NE2	1:C:216:PRO:HB3	2.30	0.45
1:X:23:ASP:HB3	1:X:29:ILE:HD11	1.98	0.45
1:X:85:GLU:HG2	1:X:136:TYR:O	2.16	0.45
1:C:17:SER:O	1:C:60:VAL:HG11	2.16	0.45
1:X:112:ILE:HG22	1:X:140:THR:HG22	1.98	0.45
1:C:123:GLU:O	1:C:127:GLU:HG3	2.17	0.45
1:C:348:ALA:HB2	1:C:352:LEU:HD23	1.99	0.45
1:C:402:ILE:CG2	1:C:403:ASP:H	2.27	0.45
1:O:265:THR:HG23	1:O:410:ASP:OD1	2.16	0.45
1:C:143:ARG:NH2	1:C:147:ASP:OD1	2.49	0.45
1:C:411:GLY:O	1:C:437:LEU:HD13	2.17	0.45
1:X:21:ILE:HG21	1:X:70:ILE:CD1	2.47	0.44
1:C:425:ASP:HB3	1:C:475:MET:HB2	1.98	0.44
1:O:404:ILE:O	1:O:429:ILE:HD13	2.17	0.44
1:B:163:PHE:CD1	1:B:164:GLY:N	2.86	0.44
1:B:383:GLN:HB3	1:B:422:PHE:CE2	2.52	0.44
1:C:56:SER:O	1:C:60:VAL:HG22	2.16	0.44
1:C:247:GLN:OE1	1:C:271:PHE:HB2	2.18	0.44
1:C:392:VAL:O	1:C:396:MET:HB2	2.18	0.44
1:C:128:LYS:NZ	1:C:201:ASP:OD2	2.46	0.44
1:O:49:ASN:HB3	1:O:52:GLU:HG3	2.00	0.44
1:O:279:GLU:OE1	1:O:281:GLN:CB	2.63	0.44
1:X:169:TRP:O	1:X:173:LYS:HG2	2.17	0.44
1:X:479:GLU:O	1:X:483:LEU:HG	2.17	0.44
1:C:126:HIS:O	1:C:130:GLY:N	2.44	0.44
1:O:415:LYS:HD3	1:O:415:LYS:O	2.18	0.44
1:X:84:ARG:H	2:X:1001:EDO:H12	1.83	0.44
1:X:279:GLU:CB	1:X:281:GLN:HG2	2.44	0.44
1:B:166:ILE:O	1:B:170:LEU:HG	2.18	0.44
1:X:327:SER:N	1:X:328:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:HB2	1:B:104:TRP:HB3	1.99	0.44
1:B:427:LEU:HD13	1:B:429:ILE:HD11	2.00	0.44
1:C:118:VAL:O	1:C:118:VAL:HG12	2.17	0.44
1:C:415:LYS:HG3	1:C:437:LEU:HD11	2.00	0.44
1:C:246:ASP:OD1	1:C:247:GLN:N	2.51	0.44
1:B:5:ASN:OD1	1:B:5:ASN:N	2.50	0.43
1:C:18:ARG:HE	1:C:20:ILE:HD11	1.82	0.43
1:C:278:GLU:OE1	1:C:298:LYS:HD3	2.18	0.43
1:B:7:VAL:HG13	1:B:77:GLY:O	2.19	0.43
1:B:246:ASP:OD1	1:B:247:GLN:N	2.51	0.43
1:X:221:ASN:ND2	1:X:294:GLY:N	2.56	0.43
1:O:273:VAL:HG22	1:O:304:GLU:HG3	2.00	0.43
1:X:225:TYR:CE2	1:X:243:MET:HE3	2.54	0.43
1:X:359:SER:HA	3:X:508:PO4:O4	2.19	0.43
1:C:110:SER:N	1:C:111:PRO:CD	2.81	0.43
1:O:229:ARG:NH1	1:O:231:TYR:OH	2.51	0.43
1:X:397:LYS:O	1:X:401:GLY:N	2.50	0.43
1:O:172:TRP:CD2	1:O:177:GLY:HA2	2.54	0.43
1:X:8:MET:CE	1:X:10:ILE:HD11	2.48	0.43
1:X:200:TRP:CG	1:X:215:LEU:HD13	2.53	0.43
1:B:171:VAL:HG21	1:B:243:MET:SD	2.59	0.43
1:B:151:GLY:HA2	1:B:154:GLU:OE2	2.19	0.43
1:B:230:SER:HB2	1:B:235:GLY:O	2.19	0.43
1:C:73:GLU:H	1:C:73:GLU:HG2	1.66	0.43
1:C:500:LYS:O	1:C:501:ALA:O	2.37	0.43
1:X:128:LYS:NZ	1:X:203:GLU:HB3	2.34	0.43
1:C:72:PRO:CG	1:C:234:TYR:HD2	2.32	0.43
1:C:334:ALA:HB2	1:C:378:VAL:HG12	2.01	0.43
1:X:283:SER:O	1:X:399:ASP:HB3	2.19	0.43
1:O:123:GLU:CD	1:O:123:GLU:H	2.21	0.42
1:X:348:ALA:HA	2:X:3133:EDO:H21	2.01	0.42
1:X:420:MET:HA	1:X:420:MET:CE	2.49	0.42
1:O:456:LYS:NZ	1:O:456:LYS:HB3	2.34	0.42
1:B:42:LYS:HG2	1:B:43:SER:N	2.34	0.42
1:C:266:TYR:CB	1:C:413:ALA:HB3	2.45	0.42
1:O:83:GLN:HG3	1:O:83:GLN:O	2.20	0.42
1:C:71:ARG:NH2	1:C:73:GLU:OE2	2.47	0.42
1:C:10:ILE:HD13	1:C:10:ILE:O	2.19	0.42
1:C:243:MET:O	1:C:244:ALA:HB2	2.19	0.42
1:X:478:GLU:HG3	1:X:479:GLU:N	2.33	0.42
1:B:262:ILE:HD11	1:B:272:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:272:ILE:HD12	1:O:392:VAL:HB	2.01	0.42
1:C:205:LEU:HD11	1:C:215:LEU:HD11	2.02	0.42
1:O:317:LEU:HD22	1:O:323:MET:HE2	2.01	0.42
1:B:190:THR:O	1:B:191:MET:CB	2.68	0.42
1:C:128:LYS:HB3	1:C:128:LYS:HE2	1.86	0.42
1:C:138:SER:O	1:C:142:VAL:HG23	2.19	0.42
1:O:229:ARG:HH11	1:O:229:ARG:HG3	1.85	0.42
1:O:408:LYS:HE2	1:O:432:GLN:NE2	2.35	0.42
1:X:225:TYR:CE1	1:X:243:MET:HG3	2.55	0.42
1:X:361:ALA:O	1:X:362:ARG:NH1	2.50	0.42
1:B:103:VAL:HG12	1:B:104:TRP:N	2.35	0.42
1:C:437:LEU:O	1:C:439:THR:N	2.45	0.42
1:B:70:ILE:CG2	1:B:71:ARG:N	2.83	0.41
1:O:449:GLY:HA3	1:O:455:TRP:CE3	2.56	0.41
1:X:72:PRO:C	1:X:74:ALA:H	2.24	0.41
1:B:375:GLU:CD	1:B:375:GLU:H	2.24	0.41
1:C:72:PRO:HB2	1:C:236:SER:OG	2.21	0.41
1:C:116:LEU:HD11	1:C:208:LEU:HD21	2.01	0.41
1:C:414:ALA:HB3	1:C:437:LEU:HD22	2.01	0.41
1:C:16:SER:HB3	1:C:35:GLU:HG2	2.03	0.41
1:C:70:ILE:HG22	1:C:71:ARG:N	2.35	0.41
1:C:370:ARG:HG3	1:C:370:ARG:NH1	2.36	0.41
1:O:200:TRP:CG	1:O:215:LEU:HD13	2.56	0.41
1:B:23:ASP:HB3	1:B:29:ILE:CD1	2.51	0.41
1:C:11:ASP:HA	1:C:81:THR:HG22	2.02	0.41
1:C:80:ILE:O	1:C:243:MET:HA	2.20	0.41
1:C:200:TRP:CD2	1:C:215:LEU:HD13	2.56	0.41
1:C:402:ILE:CG2	1:C:403:ASP:N	2.79	0.41
1:O:429:ILE:HG22	1:O:430:ASP:N	2.36	0.41
1:X:251:LEU:HA	1:X:263:LYS:HD3	2.01	0.41
1:B:81:THR:OG1	1:B:246:ASP:HA	2.21	0.41
1:B:182:THR:HA	1:B:243:MET:HE1	2.03	0.41
1:C:81:THR:HA	1:C:244:ALA:O	2.21	0.41
1:C:163:PHE:CD1	1:C:164:GLY:N	2.88	0.41
1:O:181:VAL:HG23	1:O:217:GLU:O	2.21	0.40
1:X:256:ALA:HA	1:X:261:MET:HE2	2.01	0.40
1:B:181:VAL:HG22	1:B:182:THR:H	1.84	0.40
1:B:153:GLN:HB3	1:B:154:GLU:OE1	2.20	0.40
1:B:315:GLN:HA	1:B:315:GLN:OE1	2.22	0.40
1:B:390:LYS:HD3	1:B:484:TYR:CD1	2.57	0.40
1:C:190:THR:O	1:C:191:MET:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ILE:CG2	1:C:325:GLU:N	2.82	0.40
1:B:270:ALA:HB3	1:B:307:ILE:HB	2.03	0.40
1:C:457:ASP:C	1:C:459:ASP:N	2.75	0.40
1:O:81:THR:HA	1:O:244:ALA:O	2.21	0.40
1:O:460:GLU:O	1:O:463:SER:HB2	2.22	0.40
1:X:81:THR:HA	1:X:244:ALA:O	2.21	0.40
1:X:100:ASN:HD21	2:X:3126:EDO:H12	1.87	0.40
1:X:284:ASP:HB2	1:X:303:LEU:HD21	2.03	0.40
1:B:250:ALA:HB2	1:B:440:THR:OG1	2.22	0.40
1:C:197:LYS:O	1:C:198:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	497/506 (98%)	467 (94%)	29 (6%)	1 (0%)	47	58
1	C	496/506 (98%)	444 (90%)	46 (9%)	6 (1%)	13	14
1	O	496/506 (98%)	475 (96%)	18 (4%)	3 (1%)	25	31
1	X	497/506 (98%)	466 (94%)	27 (5%)	4 (1%)	19	23
All	All	1986/2024 (98%)	1852 (93%)	120 (6%)	14 (1%)	22	26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	4	LYS
1	B	4	LYS
1	C	152	ALA
1	C	501	ALA
1	X	4	LYS

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Mol	Chain	Res	Type
1	X	402	ILE
1	C	341	ASN
1	X	465	ALA
1	C	124	MET
1	C	280	PRO
1	O	464	MET
1	X	466	GLU
1	C	438	GLU
1	O	467	GLU

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	B	400/410 (98%)	389 (97%)	11 (3%)	43	60
1	C	402/410 (98%)	390 (97%)	12 (3%)	41	57
1	O	403/410 (98%)	391 (97%)	12 (3%)	41	57
1	X	402/410 (98%)	393 (98%)	9 (2%)	52	69
All	All	1607/1640 (98%)	1563 (97%)	44 (3%)	44	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	18	ARG
1	O	67	GLU
1	O	117	LYS
1	O	124	MET
1	O	202	GLN
1	O	263	LYS
1	O	279	GLU
1	O	282	LEU
1	O	303	LEU
1	O	370	ARG
1	O	497	PHE

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Mol	Chain	Res	Type
1	X	12	GLN
1	X	42	LYS
1	X	67	GLU
1	X	83	GLN
1	X	331	GLU
1	X	340	ASP
1	X	370	ARG
1	X	478	GLU
1	X	481	ASP
1	B	12	GLN
1	B	107	ARG
1	B	154	GLU
1	B	157	ASP
1	B	306	SER
1	B	315	GLN
1	B	355	PRO
1	B	360	GLU
1	B	469	GLN
1	B	478	GLU
1	B	481	ASP
1	C	10	ILE
1	C	12	GLN
1	C	234	TYR
1	C	254	GLN
1	C	263	LYS
1	C	281	GLN
1	C	325	GLU
1	C	338	LYS
1	C	341	ASN
1	C	355	PRO
1	C	461	LEU
1	C	466	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	O	33	GLN
1	O	126	HIS
1	O	178	GLN
1	O	180	HIS
1	O	196	HIS

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Mol	Chain	Res	Type
1	O	202	GLN
1	O	221	ASN
1	O	285	ASN
1	O	421	GLN
1	O	489	GLN
1	X	12	GLN
1	X	58	GLN
1	X	83	GLN
1	X	178	GLN
1	X	180	HIS
1	X	202	GLN
1	X	221	ASN
1	X	264	ASN
1	X	341	ASN
1	X	489	GLN
1	B	12	GLN
1	B	55	ASN
1	B	58	GLN
1	B	178	GLN
1	B	264	ASN
1	B	383	GLN
1	B	495	GLN
1	C	12	GLN
1	C	33	GLN
1	C	96	GLN
1	C	126	HIS
1	C	148	ASN
1	C	202	GLN
1	C	209	ASN
1	C	221	ASN
1	C	254	GLN
1	C	285	ASN
1	C	329	GLN
1	C	383	GLN
1	C	423	GLN
1	C	489	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	EDO	O	1000	-	3,3,3	0.79	0	2,2,2	0.25	0
2	EDO	X	3126	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	B	3130	-	3,3,3	0.56	0	2,2,2	0.27	0
2	EDO	B	3131	-	3,3,3	0.48	0	2,2,2	0.31	0
3	PO4	O	509	-	4,4,4	1.38	0	6,6,6	0.42	0
2	EDO	X	3133	-	3,3,3	0.58	0	2,2,2	0.23	0
3	PO4	B	507	-	4,4,4	1.62	0	6,6,6	0.42	0
3	PO4	X	508	-	4,4,4	1.42	0	6,6,6	0.41	0
2	EDO	X	3132	-	3,3,3	0.54	0	2,2,2	0.33	0
2	EDO	B	1002	-	3,3,3	0.53	0	2,2,2	0.29	0
3	PO4	O	508	-	4,4,4	1.22	0	6,6,6	0.46	0
2	EDO	X	1001	-	3,3,3	0.60	0	2,2,2	0.31	0
3	PO4	O	507	-	4,4,4	1.61	0	6,6,6	0.44	0
2	EDO	C	1003	-	3,3,3	0.70	0	2,2,2	0.21	0
3	PO4	C	507	-	4,4,4	1.56	0	6,6,6	0.42	0
2	EDO	X	3125	-	3,3,3	0.53	0	2,2,2	0.31	0
3	PO4	X	507	-	4,4,4	1.61	0	6,6,6	0.43	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	EDO	O	1000	-	-	1/1/1/1	-
2	EDO	X	3126	-	-	1/1/1/1	-
2	EDO	B	3130	-	-	1/1/1/1	-
2	EDO	B	3131	-	-	1/1/1/1	-
2	EDO	X	3133	-	-	0/1/1/1	-
2	EDO	X	3132	-	-	1/1/1/1	-
2	EDO	B	1002	-	-	0/1/1/1	-
2	EDO	X	1001	-	-	1/1/1/1	-
2	EDO	C	1003	-	-	1/1/1/1	-
2	EDO	X	3125	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	1001	EDO	O1-C1-C2-O2
2	B	3130	EDO	O1-C1-C2-O2
2	B	3131	EDO	O1-C1-C2-O2
2	O	1000	EDO	O1-C1-C2-O2
2	X	3126	EDO	O1-C1-C2-O2
2	X	3132	EDO	O1-C1-C2-O2
2	C	1003	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	3126	EDO	1	0
2	X	3133	EDO	5	0
3	X	508	PO4	2	0
2	X	3132	EDO	3	0
2	B	1002	EDO	1	0
2	X	1001	EDO	1	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^{th} 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	B	499/506 (98%)	-0.05	6 (1%) 79 83	33, 49, 74, 94	0
1	C	498/506 (98%)	0.13	16 (3%) 47 54	37, 60, 87, 111	0
1	O	498/506 (98%)	-0.08	5 (1%) 82 86	24, 43, 70, 91	0
1	X	499/506 (98%)	-0.03	9 (1%) 68 74	28, 44, 71, 95	0
All	All	1994/2024 (98%)	-0.01	36 (1%) 68 74	24, 49, 78, 111	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	4.8
1	B	3	GLU	4.2
1	X	281	GLN	4.1
1	B	465	ALA	3.8
1	C	281	GLN	3.7
1	X	501	ALA	3.5
1	C	402	ILE	3.5
1	X	338	LYS	3.4
1	C	338	LYS	3.4
1	O	234	TYR	3.3
1	O	338	LYS	3.2
1	C	206	ASP	3.2
1	X	437	LEU	3.2
1	C	478	GLU	3.2
1	X	466	GLU	3.2
1	C	437	LEU	3.1
1	C	283	SER	3.1
1	B	331	GLU	3.0
1	B	332	GLU	2.9
1	O	281	GLN	2.9
1	C	282	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	X	282	LEU	2.7
1	O	280	PRO	2.7
1	X	465	ALA	2.7
1	B	466	GLU	2.6
1	B	338	LYS	2.5
1	C	339	GLY	2.4
1	O	282	LEU	2.3
1	C	459	ASP	2.3
1	C	256	ALA	2.2
1	X	402	ILE	2.2
1	C	401	GLY	2.1
1	C	159	GLY	2.1
1	C	466	GLU	2.0
1	C	438	GLU	2.0
1	X	340	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	EDO	B	3130	4/4	0.79	0.14	58,62,63,63	0
2	EDO	X	3133	4/4	0.88	0.25	41,43,49,52	0
2	EDO	X	3126	4/4	0.91	0.14	53,59,63,63	0
3	PO4	O	508	5/5	0.91	0.31	46,49,58,60	0
2	EDO	X	3132	4/4	0.92	0.10	40,40,44,47	0
3	PO4	O	509	5/5	0.92	0.34	56,64,70,74	0
2	EDO	O	1000	4/4	0.93	0.24	28,32,32,34	0
2	EDO	X	1001	4/4	0.93	0.22	40,42,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	X	3125	4/4	0.94	0.12	40,41,43,44	0
2	EDO	C	1003	4/4	0.94	0.15	41,43,48,52	0
3	PO4	X	508	5/5	0.94	0.37	56,59,70,72	0
3	PO4	X	507	5/5	0.95	0.12	51,60,66,67	0
2	EDO	B	3131	4/4	0.96	0.13	58,60,60,64	0
2	EDO	B	1002	4/4	0.96	0.22	37,39,43,46	0
3	PO4	B	507	5/5	0.97	0.10	51,64,69,72	0
3	PO4	C	507	5/5	0.97	0.11	63,68,74,75	0
3	PO4	O	507	5/5	0.98	0.14	58,58,63,69	0

6.5 Other polymers (i)

There are no such residues in this entry.