Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 PM GMT

PDB ID	:	4UPD
Title	:	Open conformation of O. piceae sterol esterase mutant I544W
Authors	:	Gutierrez-Fernandez, J.; Vaquero, M.E.; Prieto, A.; Barriuso, J.; Gonzalez, M.J.; Hermoso, J.A.
Deposited on	:	2014-06-16
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:

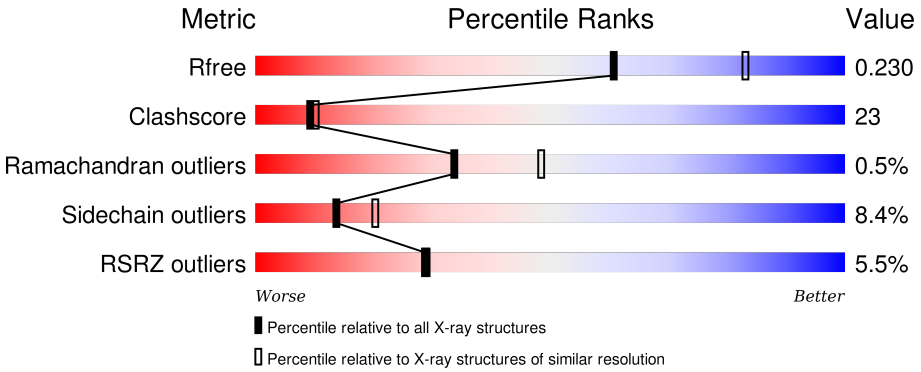
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 <=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	545	86% 11%
1	B	545	11% 46% 46% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGE	A	1551	-	-	-	X
4	NAG	A	1553	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8706 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.

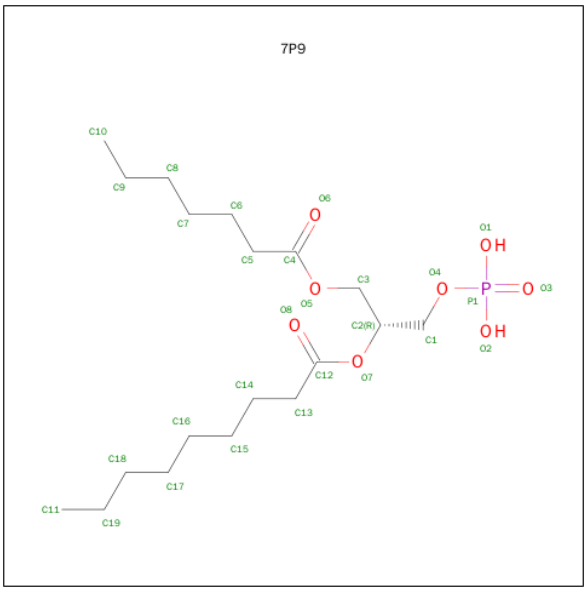
- Molecule 1 is a protein called STEROL ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4137	2676	664	787	10			
1	B	537	Total	C	N	O	S	0	0	0
			4126	2667	663	786	10			

There are 18 discrepancies between the modelled and reference sequences:

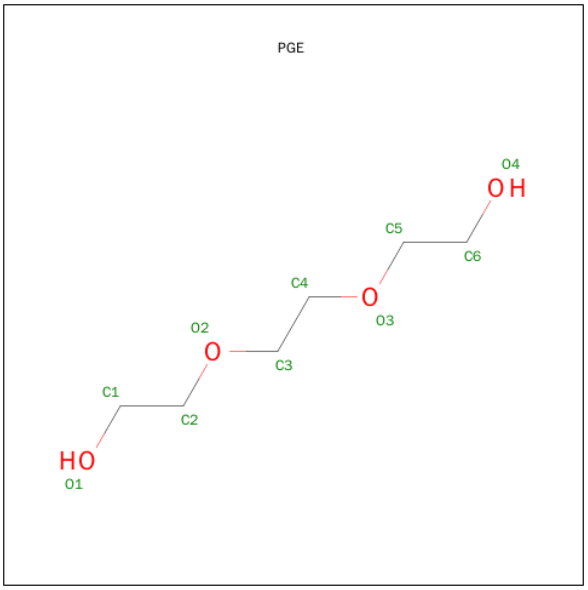
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLU	-	EXPRESSION TAG	UNP Q2TFW1
A	6	ALA	-	EXPRESSION TAG	UNP Q2TFW1
A	7	GLU	-	EXPRESSION TAG	UNP Q2TFW1
A	8	ALA	-	EXPRESSION TAG	UNP Q2TFW1
A	9	TYR	-	EXPRESSION TAG	UNP Q2TFW1
A	10	VAL	-	EXPRESSION TAG	UNP Q2TFW1
A	11	GLU	-	EXPRESSION TAG	UNP Q2TFW1
A	12	PHE	-	EXPRESSION TAG	UNP Q2TFW1
A	544	TRP	ILE	ENGINEERED MUTATION	UNP Q2TFW1
B	5	GLU	-	EXPRESSION TAG	UNP Q2TFW1
B	6	ALA	-	EXPRESSION TAG	UNP Q2TFW1
B	7	GLU	-	EXPRESSION TAG	UNP Q2TFW1
B	8	ALA	-	EXPRESSION TAG	UNP Q2TFW1
B	9	TYR	-	EXPRESSION TAG	UNP Q2TFW1
B	10	VAL	-	EXPRESSION TAG	UNP Q2TFW1
B	11	GLU	-	EXPRESSION TAG	UNP Q2TFW1
B	12	PHE	-	EXPRESSION TAG	UNP Q2TFW1
B	544	TRP	ILE	ENGINEERED MUTATION	UNP Q2TFW1

- Molecule 2 is [(2R)-2-HEPTANOYLOXY-3-PHOSPHONOOXY-PROPYL] NONANOATE (three-letter code: 7P9) (formula: $C_{19}H_{37}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			28	19	8	1		
2	B	1	Total	C	O	P	0	0
			28	19	8	1		

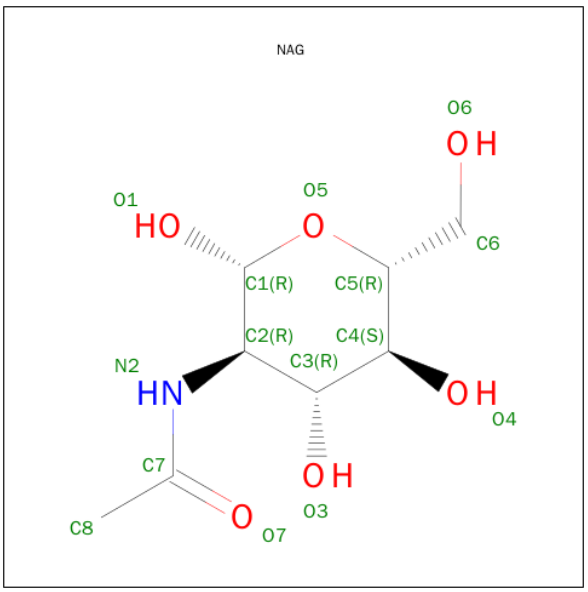
- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

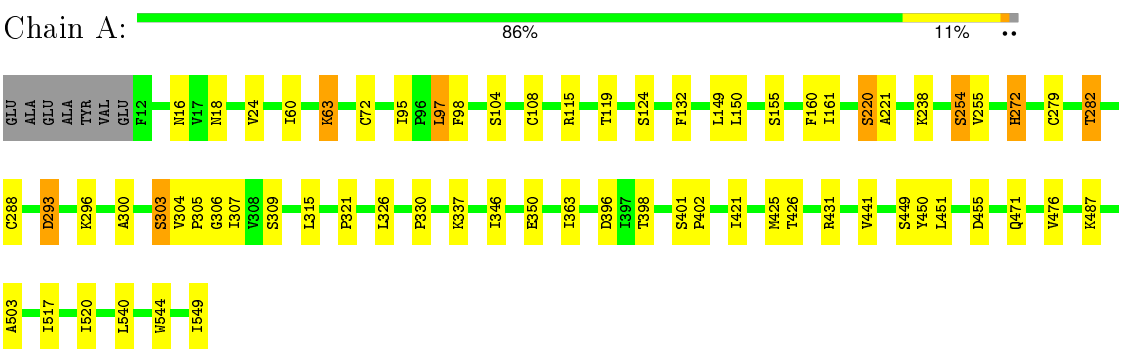
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	286	Total O 286 286	0	0
5	B	49	Total O 49 49	0	0

3 Residue-property plots (i)

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.

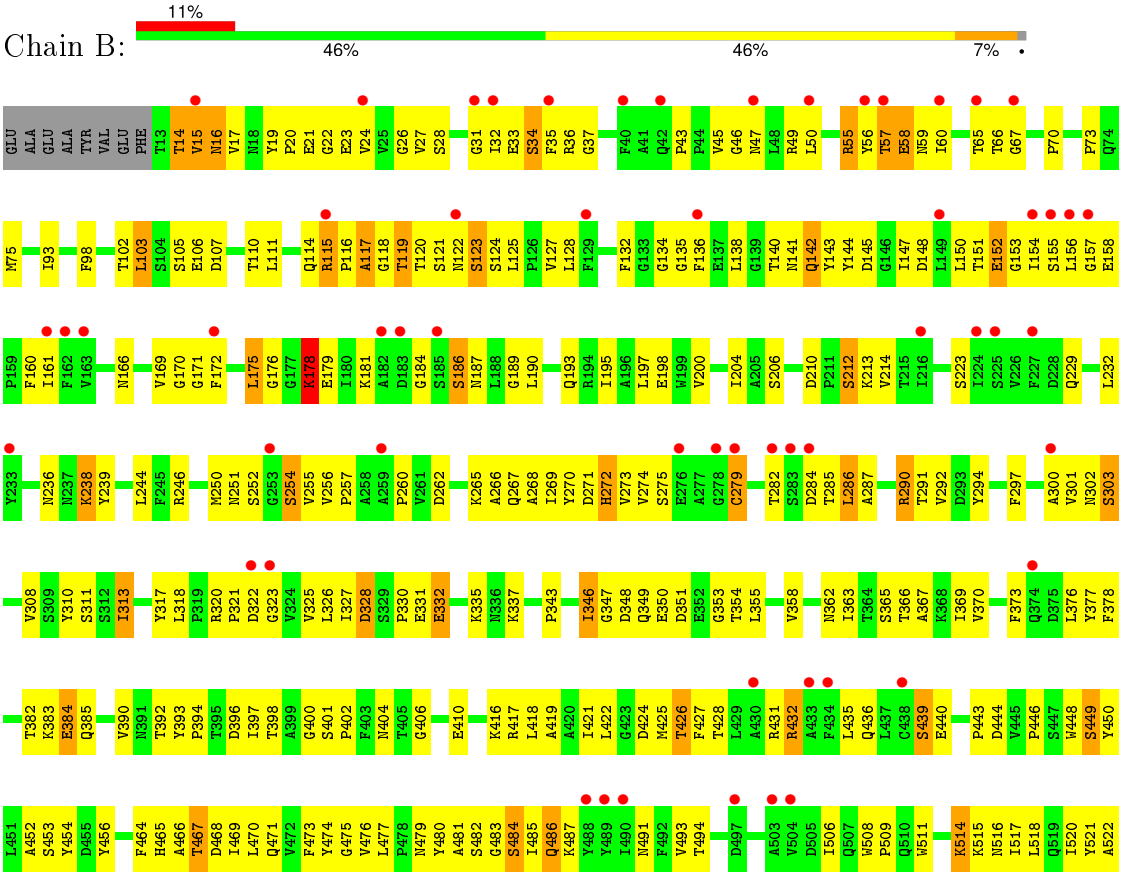
- Molecule 1: STEROL ESTERASE

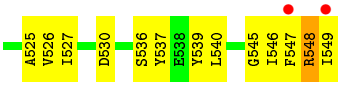
Chain A:



- Molecule 1: STEROL ESTERASE

Chain B:




A525
V526
I527
D530
S536
Y537
E538
Y539
L540
G545
I546
F547
R548
I549

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	164.86Å 164.86Å 94.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.29 – 2.40 58.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.29-2.40) 99.8 (58.29-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.248 0.208 , 0.230	Depositor DCC
R_{free} test set	2400 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.1	EDS
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49288 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.375 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: PGE, NAG, 7P9

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	1.44	0/4243	0.75	0/5787
1	B	0.94	0/4231	0.76	0/5771
All	All	1.22	0/8474	0.75	0/11558

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	VAL	Peptide
1	B	212	SER	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	4137	0	4053	41	1
1	B	4126	0	4040	329	0
2	A	28	0	37	7	0
2	B	28	0	37	9	0
3	A	10	0	14	1	0
4	A	28	0	26	1	0
4	B	14	0	13	2	0
5	A	286	0	0	4	0
5	B	49	0	0	7	0
All	All	8706	0	8220	378	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 23.

All (378) 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:366:THR:CA	1:B:369:ILE:HD13	1.45	1.40
1:B:210:ASP:OD2	1:B:213:LYS:HE2	1.24	1.34
1:B:158:GLU:OE1	1:B:494:THR:CB	1.77	1.31
1:B:482:SER:O	1:B:486:GLN:CG	1.82	1.26
1:B:269:ILE:O	1:B:273:VAL:HG23	1.30	1.25
1:B:158:GLU:OE1	1:B:494:THR:HB	1.27	1.24
1:B:366:THR:O	1:B:370:VAL:HG23	1.07	1.20
1:B:260:PRO:HB2	1:B:262:ASP:OD1	1.42	1.18
1:B:210:ASP:OD2	1:B:213:LYS:CE	1.92	1.16
1:B:443:PRO:O	1:B:444:ASP:HB3	1.44	1.16
1:B:350:GLU:OE1	1:B:453:SER:OG	1.62	1.15
1:B:480:TYR:O	1:B:484:SER:OG	1.65	1.12
1:B:300:ALA:O	1:B:303:SER:OG	1.66	1.12
1:B:366:THR:O	1:B:370:VAL:CG2	1.99	1.10
1:B:175:LEU:HD12	1:B:176:GLY:H	1.13	1.10
1:B:366:THR:CA	1:B:369:ILE:CD1	2.32	1.07
1:B:116:PRO:HB3	1:B:154:ILE:HD11	1.08	1.07
1:B:366:THR:HA	1:B:369:ILE:CD1	1.83	1.07
1:B:482:SER:O	1:B:486:GLN:HG2	1.49	1.07
1:B:116:PRO:CB	1:B:154:ILE:HD11	1.85	1.06
1:B:15:VAL:O	1:B:26:GLY:N	1.89	1.06
1:B:393:TYR:OH	1:B:424:ASP:OD2	1.73	1.05
1:A:72:CYS:SG	1:A:108:CYS:CB	2.44	1.05
1:B:15:VAL:HG13	1:B:16:ASN:CG	1.76	1.04
1:A:72:CYS:SG	1:A:108:CYS:SG	1.15	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PRO:HB3	1:B:154:ILE:CD1	1.88	1.03
1:B:396:ASP:OD2	1:B:398:THR:OG1	1.77	1.03
1:B:349:GLN:OE1	1:B:452:ALA:HB3	1.56	1.02
1:B:385:GLN:HB3	1:B:539:TYR:OH	1.57	1.02
1:B:482:SER:O	1:B:486:GLN:HG3	1.58	1.01
1:B:158:GLU:OE1	1:B:494:THR:CG2	2.08	1.00
1:B:323:GLY:HA2	1:B:327:ILE:HA	1.41	0.99
1:B:286:LEU:HD11	1:B:290:ARG:NH2	1.75	0.99
1:B:148:ASP:HA	1:B:151:THR:HB	1.42	0.98
1:B:514:LYS:HG3	1:B:516:ASN:ND2	1.78	0.97
1:B:143:TYR:O	1:B:474:TYR:OH	1.80	0.96
1:B:179:GLU:N	1:B:179:GLU:OE1	1.98	0.95
1:B:141:ASN:CG	1:B:166:ASN:ND2	2.21	0.94
1:B:178:LYS:HB3	1:B:179:GLU:OE1	1.70	0.92
1:B:19:TYR:HE1	1:B:21:GLU:HB2	1.33	0.91
1:B:279:CYS:O	1:B:282:THR:HG22	1.71	0.91
1:B:141:ASN:OD1	1:B:166:ASN:ND2	2.03	0.91
2:B:1550:7P9:H31C	2:B:1550:7P9:H152	1.52	0.90
1:B:369:ILE:HD12	1:B:369:ILE:H	1.35	0.90
1:B:382:THR:OG1	1:B:384:GLU:CG	2.20	0.89
1:A:293:ASP:OD1	5:A:2190:HOH:O	1.91	0.88
1:B:323:GLY:CA	1:B:327:ILE:HA	2.03	0.88
1:B:271:ASP:O	1:B:274:VAL:HG22	1.72	0.88
1:B:19:TYR:CE1	1:B:21:GLU:HB2	2.09	0.87
1:A:306:GLY:O	1:A:309:SER:OG	1.91	0.87
1:B:141:ASN:CG	1:B:166:ASN:HD21	1.77	0.87
1:B:382:THR:OG1	1:B:384:GLU:HG3	1.74	0.87
1:B:232:LEU:HD11	1:B:325:VAL:HG12	1.56	0.87
1:B:331:GLU:OE2	1:B:548:ARG:NH2	2.08	0.85
1:B:439:SER:OG	1:B:511:TRP:HZ3	1.58	0.85
1:B:366:THR:HA	1:B:369:ILE:HD13	0.87	0.85
1:B:170:GLY:HA2	1:B:317:TYR:CD2	2.12	0.84
1:B:178:LYS:HB2	1:B:267:GLN:OE1	1.76	0.84
1:B:256:VAL:O	1:B:330:PRO:HG2	1.77	0.84
1:B:189:GLY:O	1:B:193:GLN:HG3	1.76	0.84
1:A:97:LEU:HD23	1:A:98:PHE:CE1	2.11	0.83
1:B:15:VAL:HG13	1:B:16:ASN:CB	2.08	0.83
1:B:286:LEU:O	1:B:286:LEU:HD12	1.76	0.83
1:B:93:ILE:HA	1:B:98:PHE:HD2	1.43	0.83
1:B:175:LEU:HD12	1:B:176:GLY:N	1.93	0.83
1:B:110:THR:OG1	5:B:2001:HOH:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1550:7P9:H152	2:A:1550:7P9:H31C	1.59	0.83
1:B:346:ILE:HG12	1:B:431:ARG:HG3	1.61	0.82
1:B:349:GLN:OE1	1:B:452:ALA:CB	2.27	0.82
1:B:432:ARG:HG2	1:B:537:TYR:CE1	2.15	0.81
1:B:158:GLU:OE1	1:B:494:THR:HG21	1.79	0.81
1:B:141:ASN:ND2	1:B:166:ASN:HD22	1.79	0.80
1:B:141:ASN:ND2	1:B:166:ASN:ND2	2.30	0.80
1:B:246:ARG:NH2	1:B:493:VAL:O	2.12	0.79
1:A:300:ALA:O	1:A:303:SER:HB3	1.83	0.79
1:A:72:CYS:CB	1:A:108:CYS:SG	2.72	0.77
1:B:21:GLU:OE1	1:B:56:TYR:HB2	1.85	0.77
1:B:15:VAL:HA	1:B:16:ASN:HB3	1.67	0.77
1:A:421:ILE:O	1:A:425:MET:HG2	1.85	0.77
1:B:443:PRO:O	1:B:444:ASP:CB	2.26	0.76
1:B:200:VAL:O	1:B:204:ILE:HG22	1.85	0.76
1:B:186:SER:OG	5:B:2013:HOH:O	2.04	0.76
1:A:396:ASP:OD2	1:A:398:THR:OG1	2.03	0.75
1:B:410:GLU:OE1	1:B:416:LYS:HG3	1.88	0.74
1:B:45:VAL:HG22	1:B:46:GLY:N	2.03	0.73
1:B:178:LYS:CB	1:B:179:GLU:OE1	2.37	0.73
1:B:382:THR:OG1	1:B:384:GLU:HG2	1.87	0.72
1:B:57:THR:C	1:B:58:GLU:OE2	2.20	0.72
1:B:318:LEU:HD23	1:B:318:LEU:N	2.04	0.72
1:B:286:LEU:HD11	1:B:290:ARG:HH21	1.53	0.72
1:B:265:LYS:NZ	1:B:376:LEU:O	2.23	0.72
1:B:286:LEU:CD1	1:B:290:ARG:NH2	2.50	0.72
1:B:269:ILE:HA	1:B:272:HIS:NE2	2.04	0.71
1:B:254:SER:OG	1:B:255:VAL:N	2.22	0.71
1:A:476:VAL:O	2:A:1550:7P9:H142	1.90	0.71
1:B:439:SER:HG	1:B:511:TRP:HZ3	0.76	0.70
1:B:279:CYS:O	1:B:282:THR:CG2	2.40	0.70
1:B:269:ILE:HA	1:B:272:HIS:CD2	2.25	0.70
1:B:400:GLY:HA3	1:B:416:LYS:HB3	1.74	0.69
2:A:1550:7P9:C15	2:A:1550:7P9:H31C	2.24	0.68
1:A:254:SER:OG	1:A:255:VAL:N	2.28	0.67
1:B:266:ALA:O	1:B:269:ILE:HG13	1.95	0.67
1:B:14:THR:O	1:B:15:VAL:HG23	1.95	0.67
1:B:15:VAL:HG13	1:B:16:ASN:HB3	1.74	0.67
1:B:286:LEU:C	1:B:286:LEU:HD12	2.15	0.67
1:B:418:LEU:HD12	1:B:422:LEU:HG	1.77	0.66
1:B:347:GLY:HA3	1:B:450:TYR:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:O	1:B:273:VAL:CG2	2.25	0.66
1:B:116:PRO:O	1:B:117:ALA:CB	2.44	0.66
1:B:15:VAL:CA	1:B:16:ASN:HB3	2.26	0.66
1:B:464:PHE:O	1:B:467:THR:OG1	2.13	0.65
1:B:210:ASP:OD2	1:B:213:LYS:HE3	1.94	0.65
1:B:115:ARG:HE	1:B:119:THR:HG23	1.61	0.65
1:B:223:SER:OG	1:B:250:MET:HB3	1.97	0.65
1:B:419:ALA:O	5:B:2026:HOH:O	2.15	0.64
1:B:93:ILE:HA	1:B:98:PHE:CD2	2.30	0.64
1:B:369:ILE:CD1	1:B:369:ILE:H	2.09	0.64
1:B:435:LEU:O	1:B:439:SER:OG	2.16	0.64
1:B:439:SER:OG	1:B:511:TRP:CZ3	2.39	0.64
1:B:55:ARG:HH12	1:B:195:ILE:HG13	1.63	0.64
1:B:16:ASN:OD1	1:B:17:VAL:N	2.31	0.63
1:B:514:LYS:NZ	1:B:516:ASN:HD22	1.95	0.63
1:B:171:GLY:O	5:B:2011:HOH:O	2.14	0.63
1:A:307:ILE:HD12	1:A:315:LEU:HD21	1.81	0.63
1:B:236:ASN:OD1	1:B:238:LYS:HB2	1.99	0.63
1:B:410:GLU:OE1	1:B:410:GLU:HA	1.99	0.63
2:B:1550:7P9:H31C	2:B:1550:7P9:C15	2.26	0.62
1:A:487:LYS:HE3	1:A:503:ALA:O	1.99	0.62
1:B:55:ARG:NH1	1:B:195:ILE:HG13	2.14	0.62
1:B:481:ALA:O	1:B:485:ILE:HG13	1.99	0.62
1:B:348:ASP:OD2	1:B:428:THR:HA	1.99	0.62
1:A:304:VAL:HB	1:A:305:PRO:CD	2.30	0.62
1:B:172:PHE:H	1:B:172:PHE:HD1	1.47	0.62
1:A:304:VAL:HB	1:A:305:PRO:HD2	1.81	0.62
1:B:323:GLY:HA2	1:B:327:ILE:CA	2.25	0.61
1:A:97:LEU:CD2	1:A:98:PHE:CE1	2.83	0.61
1:B:527:ILE:H	1:B:527:ILE:HD12	1.64	0.61
1:B:19:TYR:HB2	1:B:20:PRO:HD2	1.83	0.61
1:B:156:LEU:HG	1:B:157:GLY:H	1.65	0.61
1:B:116:PRO:CG	1:B:154:ILE:HD11	2.31	0.61
1:B:198:GLU:HG2	1:B:239:TYR:CD1	2.35	0.61
1:B:15:VAL:CG1	1:B:16:ASN:CG	2.63	0.60
1:B:292:VAL:HG12	1:B:297:PHE:HB2	1.82	0.60
1:B:527:ILE:HD12	1:B:527:ILE:N	2.16	0.60
1:B:476:VAL:O	2:B:1550:7P9:H132	2.01	0.60
1:B:282:THR:CG2	1:B:285:THR:HA	2.32	0.60
1:A:401:SER:HA	1:A:402:PRO:C	2.21	0.60
1:A:60:ILE:HD12	1:A:63:LYS:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLU:HG3	1:B:385:GLN:H	1.66	0.60
1:B:525:ALA:O	1:B:526:VAL:HG12	2.01	0.60
1:B:392:THR:HB	1:B:536:SER:OG	2.02	0.59
1:B:480:TYR:HB3	1:B:522:ALA:O	2.02	0.59
1:B:75:MET:HG3	1:B:302:ASN:CG	2.23	0.59
1:B:67:GLY:HA3	5:B:2002:HOH:O	2.01	0.59
1:B:425:MET:HG2	1:B:426:THR:H	1.67	0.59
1:B:355:LEU:HD13	1:B:464:PHE:CD2	2.38	0.58
1:A:450:TYR:CD2	1:A:520:ILE:HD12	2.39	0.58
1:B:363:ILE:CG2	1:B:369:ILE:HA	2.34	0.58
1:B:382:THR:N	1:B:385:GLN:OE1	2.35	0.58
1:A:97:LEU:HD23	1:A:98:PHE:CD1	2.39	0.58
1:B:37:GLY:HA2	5:B:2001:HOH:O	2.04	0.58
1:B:404:ASN:O	1:B:456:TYR:OH	2.20	0.58
1:B:34:SER:HB3	1:B:114:GLN:HG2	1.86	0.57
1:B:511:TRP:O	1:B:515:LYS:HA	2.04	0.57
1:B:160:PHE:HD2	1:B:161:ILE:O	1.87	0.57
1:B:382:THR:HG1	1:B:385:GLN:CD	2.05	0.57
1:B:111:LEU:HD12	1:B:111:LEU:C	2.25	0.57
1:B:148:ASP:CA	1:B:151:THR:HB	2.27	0.56
1:B:483:GLY:HA2	1:B:486:GLN:HE21	1.69	0.56
1:B:274:VAL:HG23	1:B:275:SER:N	2.18	0.56
1:B:509:PRO:HB2	1:B:514:LYS:HE3	1.86	0.56
1:B:178:LYS:HE3	1:B:267:GLN:OE1	2.04	0.56
1:B:525:ALA:C	1:B:526:VAL:CG1	2.74	0.56
1:B:45:VAL:CG2	1:B:46:GLY:N	2.67	0.56
1:B:331:GLU:HG2	1:B:332:GLU:N	2.21	0.56
1:B:172:PHE:CD1	1:B:172:PHE:N	2.73	0.56
1:B:252:SER:O	1:B:427:PHE:CD2	2.59	0.56
1:B:45:VAL:HG22	1:B:46:GLY:H	1.71	0.55
1:B:469:ILE:O	1:B:473:PHE:HB3	2.05	0.55
1:B:175:LEU:CD1	1:B:269:ILE:CD1	2.85	0.55
1:B:269:ILE:HD12	1:B:270:TYR:N	2.22	0.55
1:B:432:ARG:CG	1:B:537:TYR:CE1	2.87	0.55
1:B:32:ILE:HA	1:B:115:ARG:O	2.06	0.55
1:A:455:ASP:OD1	2:A:1550:7P9:HA	2.07	0.55
2:B:1550:7P9:C3	2:B:1550:7P9:H152	2.32	0.55
1:B:385:GLN:CB	1:B:539:TYR:OH	2.43	0.54
1:B:171:GLY:HA3	1:B:301:VAL:HG11	1.89	0.54
1:B:252:SER:O	1:B:427:PHE:CE2	2.60	0.54
1:B:232:LEU:HD11	1:B:325:VAL:CG1	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:O	1:B:549:ILE:HG13	2.06	0.54
1:B:116:PRO:O	1:B:117:ALA:HB3	2.07	0.54
1:B:377:TYR:O	1:B:549:ILE:HD12	2.08	0.54
1:B:55:ARG:NH1	1:B:195:ILE:CG1	2.71	0.54
1:B:327:ILE:HG13	1:B:328:ASP:N	2.23	0.54
1:B:425:MET:CG	1:B:426:THR:N	2.70	0.54
1:A:272:HIS:CE1	5:A:2077:HOH:O	2.61	0.54
1:B:446:PRO:HB2	1:B:448:TRP:CH2	2.43	0.54
1:B:525:ALA:O	1:B:526:VAL:CG1	2.56	0.53
1:B:148:ASP:HA	1:B:151:THR:CB	2.29	0.53
1:B:418:LEU:HD12	1:B:418:LEU:O	2.09	0.53
1:B:178:LYS:HB3	1:B:179:GLU:CD	2.29	0.53
1:B:401:SER:HA	1:B:402:PRO:C	2.29	0.53
1:B:384:GLU:HG3	1:B:385:GLN:N	2.23	0.53
1:B:477:LEU:H	2:B:1550:7P9:H132	1.74	0.53
1:B:21:GLU:O	1:B:59:ASN:HA	2.09	0.52
1:B:321:PRO:HA	1:B:326:LEU:HB3	1.91	0.52
1:B:49:ARG:NE	1:B:106:GLU:OE2	2.20	0.52
1:B:366:THR:HG23	1:B:367:ALA:N	2.24	0.52
1:B:232:LEU:CD1	1:B:325:VAL:HG12	2.33	0.52
1:A:255:VAL:HG13	1:A:330:PRO:HB2	1.92	0.52
1:B:514:LYS:HG3	1:B:516:ASN:HD22	1.66	0.52
1:B:318:LEU:CD2	1:B:318:LEU:N	2.73	0.52
1:B:210:ASP:CG	1:B:213:LYS:HE2	2.17	0.52
1:B:353:GLY:HA3	1:B:419:ALA:O	2.10	0.51
1:B:471:GLN:HA	1:B:476:VAL:O	2.10	0.51
1:B:525:ALA:C	1:B:526:VAL:HG13	2.29	0.51
1:A:426:THR:HG21	3:A:1551:PGE:H6	1.92	0.51
1:B:362:ASN:HB3	1:B:363:ILE:HD13	1.92	0.51
1:B:418:LEU:CD1	1:B:422:LEU:HG	2.40	0.51
1:B:172:PHE:CE2	1:B:297:PHE:HE2	2.27	0.51
1:B:73:PRO:HG2	1:B:172:PHE:CE2	2.46	0.50
1:A:346:ILE:HG12	1:A:431:ARG:HG3	1.92	0.50
1:B:17:VAL:O	1:B:23:GLU:HG3	2.11	0.50
1:B:134:GLY:HA3	1:B:138:LEU:O	2.11	0.50
1:B:540:LEU:HD12	1:B:547:PHE:CE2	2.46	0.50
1:B:43:PRO:O	1:B:45:VAL:HG12	2.12	0.50
1:B:310:TYR:CE2	4:B:1551:NAG:C1	2.94	0.50
1:B:351:ASP:OD1	1:B:402:PRO:HA	2.12	0.50
1:B:369:ILE:HD12	1:B:369:ILE:N	2.15	0.50
1:B:120:THR:H	1:B:123:SER:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HB	1:B:214:VAL:HG22	1.93	0.50
1:B:49:ARG:HH21	1:B:106:GLU:CD	2.11	0.50
1:B:393:TYR:CD2	1:B:421:ILE:HG12	2.46	0.50
1:A:337:LYS:HG3	1:A:441:VAL:HB	1.93	0.50
1:B:15:VAL:CG1	1:B:16:ASN:HB3	2.42	0.49
1:B:200:VAL:O	1:B:204:ILE:CG2	2.58	0.49
1:B:132:PHE:CD1	1:B:132:PHE:C	2.85	0.49
1:B:153:GLY:O	1:B:156:LEU:O	2.30	0.49
1:B:477:LEU:N	2:B:1550:7P9:H132	2.28	0.49
1:B:190:LEU:HD23	1:B:193:GLN:OE1	2.13	0.49
1:B:171:GLY:HA3	1:B:301:VAL:CG1	2.42	0.49
1:A:279:CYS:O	1:A:282:THR:OG1	2.30	0.49
1:A:350:GLU:HA	1:A:451:LEU:HD11	1.95	0.49
1:B:15:VAL:CG1	1:B:16:ASN:CB	2.88	0.49
1:B:45:VAL:CG2	1:B:46:GLY:H	2.26	0.49
1:B:274:VAL:CG2	1:B:275:SER:N	2.76	0.49
2:A:1550:7P9:H141	5:A:2257:HOH:O	2.12	0.49
1:A:363:ILE:CD1	4:A:1552:NAG:H82	2.42	0.48
1:B:365:SER:O	1:B:369:ILE:N	2.40	0.48
1:B:393:TYR:O	1:B:417:ARG:NH2	2.44	0.48
1:B:509:PRO:CB	1:B:514:LYS:HE3	2.43	0.48
1:B:471:GLN:NE2	2:B:1550:7P9:O8	2.46	0.48
1:B:118:GLY:O	1:B:120:THR:HG23	2.14	0.48
1:B:308:VAL:HG12	1:B:308:VAL:O	2.12	0.48
1:B:270:TYR:O	1:B:274:VAL:HG13	2.13	0.48
1:B:476:VAL:HG12	1:B:477:LEU:HD23	1.96	0.48
1:B:15:VAL:HG13	1:B:16:ASN:OD1	2.12	0.48
1:B:144:TYR:HE1	1:B:469:ILE:HD12	1.79	0.47
1:A:455:ASP:OD1	2:A:1550:7P9:H131	2.13	0.47
1:B:251:ASN:N	1:B:251:ASN:HD22	2.12	0.47
1:B:140:THR:HG23	1:B:142:GLN:H	1.79	0.47
1:B:246:ARG:O	1:B:343:PRO:HD2	2.14	0.47
1:B:509:PRO:CB	1:B:514:LYS:CE	2.92	0.47
1:B:178:LYS:O	1:B:181:LYS:HB3	2.15	0.47
1:B:257:PRO:HB2	1:B:548:ARG:HA	1.97	0.47
1:B:271:ASP:O	1:B:274:VAL:CG2	2.54	0.47
1:B:425:MET:HG2	1:B:426:THR:N	2.30	0.47
1:B:321:PRO:N	1:B:326:LEU:HD23	2.28	0.47
1:B:197:LEU:O	1:B:200:VAL:HB	2.15	0.47
1:B:125:LEU:O	1:B:210:ASP:N	2.45	0.46
1:B:184:GLY:HA2	5:B:2013:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ILE:HD11	1:B:422:LEU:HB3	1.98	0.46
1:B:426:THR:HB	1:B:427:PHE:CD1	2.51	0.46
1:B:318:LEU:HD23	1:B:318:LEU:H	1.75	0.46
1:B:378:PHE:CD1	1:B:547:PHE:HA	2.51	0.46
1:B:145:ASP:N	1:B:474:TYR:OH	2.37	0.46
1:B:58:GLU:N	1:B:58:GLU:OE2	2.47	0.46
1:B:49:ARG:NH2	1:B:106:GLU:OE1	2.23	0.46
1:B:102:THR:C	1:B:103:LEU:HG	2.36	0.46
1:B:479:ASN:O	1:B:482:SER:OG	2.27	0.46
1:B:73:PRO:CG	1:B:172:PHE:CE2	2.99	0.46
1:B:349:GLN:HA	1:B:349:GLN:OE1	2.16	0.46
1:B:393:TYR:HA	1:B:394:PRO:HD3	1.82	0.46
1:B:128:LEU:HD23	1:B:160:PHE:CE2	2.50	0.46
1:B:509:PRO:HB3	1:B:514:LYS:HE2	1.98	0.45
1:B:19:TYR:N	1:B:22:GLY:O	2.43	0.45
1:B:390:VAL:O	1:B:417:ARG:NH2	2.49	0.45
1:B:468:ASP:N	1:B:468:ASP:OD1	2.41	0.45
1:B:190:LEU:HA	1:B:190:LEU:HD23	1.75	0.45
1:B:473:PHE:C	1:B:473:PHE:CD1	2.89	0.45
1:A:132:PHE:C	1:A:132:PHE:CD1	2.90	0.45
1:B:73:PRO:HG2	1:B:172:PHE:CD2	2.52	0.45
1:B:175:LEU:CD1	1:B:269:ILE:HD12	2.46	0.45
1:B:31:GLY:O	1:B:117:ALA:HB2	2.17	0.45
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.67	0.45
1:B:366:THR:HB	1:B:417:ARG:HH12	1.81	0.45
1:B:158:GLU:OE1	1:B:494:THR:OG1	2.31	0.45
1:B:31:GLY:C	1:B:117:ALA:HB2	2.37	0.45
1:A:425:MET:O	5:A:2248:HOH:O	2.21	0.45
1:A:449:SER:HB3	1:A:517:ILE:HG22	1.98	0.45
1:A:115:ARG:HD2	1:A:119:THR:HB	1.99	0.45
1:B:158:GLU:CG	1:B:494:THR:HG21	2.46	0.45
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.78	0.45
1:A:16:ASN:HB2	1:A:24:VAL:O	2.15	0.45
1:B:354:THR:O	1:B:358:VAL:HG23	2.16	0.45
1:B:465:HIS:O	1:B:466:ALA:HB3	2.17	0.45
1:B:363:ILE:HG22	1:B:369:ILE:HG13	1.99	0.45
1:B:310:TYR:CZ	4:B:1551:NAG:H5	2.52	0.45
1:B:294:TYR:C	1:B:294:TYR:CD1	2.89	0.45
1:B:508:TRP:CD2	1:B:518:LEU:HD12	2.52	0.44
1:B:156:LEU:HG	1:B:157:GLY:N	2.32	0.44
1:B:320:ARG:C	1:B:326:LEU:HD23	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PHE:HA	1:B:377:TYR:HB2	1.98	0.44
1:A:150:LEU:HD11	1:A:160:PHE:O	2.17	0.44
1:B:15:VAL:CG1	1:B:16:ASN:OD1	2.66	0.44
1:B:432:ARG:HA	1:B:435:LEU:HD12	2.00	0.44
1:B:140:THR:HG21	1:B:142:GLN:OE1	2.17	0.44
1:B:151:THR:O	1:B:155:SER:N	2.47	0.44
2:B:1550:7P9:H31C	2:B:1550:7P9:C14	2.48	0.43
1:B:321:PRO:CA	1:B:326:LEU:HD23	2.48	0.43
1:B:36:ARG:O	1:B:65:THR:HB	2.18	0.43
2:B:1550:7P9:H72C	2:B:1550:7P9:C16	2.48	0.43
1:B:398:THR:HG22	1:B:406:GLY:HA2	2.00	0.43
1:B:213:LYS:HA	1:B:246:ARG:HD3	2.01	0.43
1:B:158:GLU:OE2	1:B:491:ASN:OD1	2.36	0.43
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.72	0.43
1:B:517:ILE:HG23	1:B:530:ASP:HB2	2.00	0.43
1:B:349:GLN:NE2	1:B:468:ASP:HB3	2.34	0.43
1:A:321:PRO:HA	1:A:326:LEU:HB3	2.00	0.43
1:B:473:PHE:CD1	1:B:473:PHE:O	2.72	0.43
1:A:346:ILE:O	1:A:449:SER:HA	2.19	0.43
1:B:323:GLY:C	1:B:327:ILE:HA	2.39	0.42
1:A:471:GLN:OE1	2:A:1550:7P9:O8	2.36	0.42
1:B:432:ARG:HG2	1:B:537:TYR:CD1	2.52	0.42
1:B:135:GLY:O	1:B:136:PHE:HB2	2.18	0.42
1:B:482:SER:O	1:B:486:GLN:CD	2.53	0.42
1:B:14:THR:C	1:B:15:VAL:HG23	2.39	0.42
1:B:152:GLU:HA	1:B:155:SER:HB3	2.01	0.42
1:B:158:GLU:CD	1:B:494:THR:HG21	2.40	0.42
1:B:35:PHE:CD1	1:B:35:PHE:N	2.88	0.42
1:B:520:ILE:HG22	1:B:521:TYR:O	2.19	0.42
1:B:514:LYS:HZ1	1:B:516:ASN:HD22	1.67	0.42
1:B:172:PHE:CE2	1:B:297:PHE:CE2	3.07	0.42
1:B:514:LYS:HG3	1:B:516:ASN:CG	2.38	0.42
1:B:75:MET:HG3	1:B:302:ASN:OD1	2.19	0.42
1:B:115:ARG:HB2	1:B:119:THR:HG21	2.02	0.42
1:B:27:VAL:HG13	1:B:27:VAL:O	2.19	0.42
1:B:176:GLY:O	1:B:270:TYR:HB2	2.20	0.41
1:B:321:PRO:HA	1:B:326:LEU:HD23	2.01	0.41
1:B:287:ALA:HA	1:B:290:ARG:NH1	2.35	0.41
1:B:431:ARG:HD2	1:B:449:SER:OG	2.21	0.41
1:B:150:LEU:HD21	1:B:160:PHE:O	2.20	0.41
1:B:448:TRP:CE3	1:B:448:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HB3	1:A:221:ALA:H	1.63	0.41
1:B:16:ASN:OD1	1:B:17:VAL:CG2	2.69	0.41
1:B:450:TYR:HB3	1:B:508:TRP:CZ2	2.55	0.41
1:B:28:SER:HB2	1:B:33:GLU:HG2	2.01	0.41
1:B:346:ILE:O	1:B:449:SER:HA	2.20	0.41
1:B:58:GLU:N	1:B:58:GLU:CD	2.73	0.41
1:B:436:GLN:NE2	1:B:440:GLU:OE2	2.45	0.41
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.80	0.41
1:B:70:PRO:C	1:B:142:GLN:NE2	2.74	0.41
1:B:17:VAL:O	1:B:24:VAL:N	2.41	0.41
1:B:545:GLY:O	1:B:548:ARG:HG2	2.21	0.41
1:B:431:ARG:HB3	1:B:431:ARG:HE	1.73	0.41
1:B:115:ARG:NE	1:B:119:THR:HG23	2.31	0.41
1:B:527:ILE:CD1	1:B:527:ILE:N	2.82	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.88	0.41
1:B:268:ALA:O	1:B:272:HIS:CD2	2.74	0.40
1:B:454:TYR:CD1	1:B:471:GLN:HG2	2.57	0.40
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.96	0.40
1:B:16:ASN:OD1	1:B:17:VAL:HG23	2.21	0.40
1:B:300:ALA:C	1:B:303:SER:OG	2.51	0.40
1:B:471:GLN:O	1:B:475:GLY:HA2	2.22	0.40
1:B:322:ASP:OD1	1:B:322:ASP:N	2.54	0.40
1:B:509:PRO:HB2	1:B:514:LYS:CE	2.52	0.40
1:B:105:SER:C	1:B:107:ASP:N	2.75	0.40
1:B:187:ASN:O	1:B:190:LEU:HB2	2.22	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:A:18:ASN:OD1	1:A:296:LYS:NZ[7_554]	1.87	0.33

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	536/545 (98%)	523 (98%)	12 (2%)	1 (0%)	52 69
1	B	535/545 (98%)	512 (96%)	19 (4%)	4 (1%)	26 38
All	All	1071/1090 (98%)	1035 (97%)	31 (3%)	5 (0%)	34 48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	ALA
1	B	178	LYS
1	B	254	SER
1	B	16	ASN
1	A	254	SER

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	443/448 (99%)	425 (96%)	18 (4%)	37 57
1	B	442/448 (99%)	386 (87%)	56 (13%)	5 6
All	All	885/896 (99%)	811 (92%)	74 (8%)	14 20

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	95	ILE
1	A	97	LEU
1	A	104	SER
1	A	124	SER
1	A	149	LEU
1	A	155	SER
1	A	161	ILE

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Mol	Chain	Res	Type
1	A	220	SER
1	A	238	LYS
1	A	272	HIS
1	A	282	THR
1	A	288	CYS
1	A	293	ASP
1	A	303	SER
1	A	540	LEU
1	A	544	TRP
1	A	549	ILE
1	B	14	THR
1	B	34	SER
1	B	47	ASN
1	B	55	ARG
1	B	57	THR
1	B	58	GLU
1	B	60	ILE
1	B	66	THR
1	B	103	LEU
1	B	115	ARG
1	B	119	THR
1	B	121	SER
1	B	122	ASN
1	B	123	SER
1	B	124	SER
1	B	142	GLN
1	B	147	ILE
1	B	152	GLU
1	B	169	VAL
1	B	175	LEU
1	B	178	LYS
1	B	186	SER
1	B	206	SER
1	B	212	SER
1	B	229	GLN
1	B	238	LYS
1	B	272	HIS
1	B	279	CYS
1	B	284	ASP
1	B	286	LEU
1	B	290	ARG
1	B	291	THR

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Mol	Chain	Res	Type
1	B	303	SER
1	B	311	SER
1	B	313	ILE
1	B	328	ASP
1	B	332	GLU
1	B	335	LYS
1	B	337	LYS
1	B	346	ILE
1	B	383	LYS
1	B	384	GLU
1	B	397	ILE
1	B	426	THR
1	B	432	ARG
1	B	439	SER
1	B	449	SER
1	B	467	THR
1	B	470	LEU
1	B	484	SER
1	B	486	GLN
1	B	487	LYS
1	B	506	ILE
1	B	514	LYS
1	B	546	ILE
1	B	548	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	166	ASN
1	B	251	ASN
1	B	272	HIS
1	B	404	ASN
1	B	471	GLN
1	B	486	GLN
1	B	507	GLN
1	B	516	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	7P9	A	1550	-	27,27,27	1.72	5 (18%)	30,32,32	2.08	7 (23%)
3	PGE	A	1551	-	9,9,9	1.13	0	8,8,8	0.66	0
4	NAG	A	1552	1	14,14,15	0.28	0	15,19,21	0.53	0
4	NAG	A	1553	1	14,14,15	0.44	0	15,19,21	0.74	0
2	7P9	B	1550	-	27,27,27	1.82	5 (18%)	30,32,32	1.88	5 (16%)
4	NAG	B	1551	1	14,14,15	0.83	1 (7%)	15,19,21	2.18	3 (20%)

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	7P9	A	1550	-	-	1/29/29/29	0/0/0/0
3	PGE	A	1551	-	-	0/7/7/7	0/0/0/0
4	NAG	A	1552	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1553	1	-	0/6/23/26	0/1/1/1
2	7P9	B	1550	-	-	0/29/29/29	0/0/0/0
4	NAG	B	1551	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1550	7P9	O7-C2	-2.25	1.40	1.46
2	A	1550	7P9	O7-C2	-2.08	1.41	1.46
4	B	1551	NAG	C1-C2	-2.01	1.49	1.52
2	A	1550	7P9	O7-C12	2.58	1.42	1.34
2	A	1550	7P9	O5-C4	2.61	1.41	1.33
2	B	1550	7P9	O7-C12	2.70	1.42	1.34
2	B	1550	7P9	O5-C4	2.93	1.42	1.33
2	A	1550	7P9	O6-C4	4.71	1.36	1.22
2	B	1550	7P9	O6-C4	5.20	1.38	1.22
2	A	1550	7P9	O8-C12	5.72	1.39	1.22
2	B	1550	7P9	O8-C12	5.87	1.40	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1550	7P9	O7-C12-O8	-6.25	106.91	123.67
4	B	1551	NAG	C1-O5-C5	-5.66	105.07	112.25
2	B	1550	7P9	O5-C4-O6	-5.27	109.88	123.49
2	A	1550	7P9	O5-C4-O6	-5.22	110.02	123.49
2	B	1550	7P9	O7-C12-O8	-4.99	110.28	123.67
2	A	1550	7P9	O8-C12-C13	-4.48	105.81	123.72
2	B	1550	7P9	O6-C4-C5	-4.24	106.76	123.72
2	B	1550	7P9	O8-C12-C13	-4.11	107.30	123.72
2	A	1550	7P9	O6-C4-C5	-3.37	110.25	123.72
2	A	1550	7P9	C3-C2-C1	-2.75	105.64	112.07
2	A	1550	7P9	C3-O5-C4	-2.68	109.35	116.85
4	B	1551	NAG	O4-C4-C3	-2.39	104.95	110.34
2	B	1550	7P9	O7-C12-C13	-2.32	106.49	111.53
2	A	1550	7P9	O5-C3-C2	-2.23	102.68	108.69
4	B	1551	NAG	C4-C3-C2	4.64	118.44	111.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1550	7P9	C2-O7-C12-O8

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1550	7P9	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	PGE	1	0
4	A	1552	NAG	1	0
2	B	1550	7P9	9	0
4	B	1551	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	538/545 (98%)	-0.32	0 100 100	22, 35, 46, 62	0
1	B	537/545 (98%)	0.58	59 (10%) 7 7	42, 72, 103, 116	0
All	All	1075/1090 (98%)	0.13	59 (5%) 29 29	22, 46, 96, 116	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	ALA	6.7
1	B	225	SER	6.2
1	B	50	LEU	5.4
1	B	156	LEU	4.8
1	B	430	ALA	4.5
1	B	24	VAL	4.4
1	B	149	LEU	4.3
1	B	547	PHE	4.2
1	B	47	ASN	4.1
1	B	155	SER	3.9
1	B	172	PHE	3.7
1	B	183	ASP	3.7
1	B	154	ILE	3.6
1	B	323	GLY	3.5
1	B	322	ASP	3.4
1	B	57	THR	3.3
1	B	490	ILE	3.3
1	B	279	CYS	3.3
1	B	282	THR	3.2
1	B	65	THR	3.0
1	B	434	PHE	2.9
1	B	122	ASN	2.9
1	B	497	ASP	2.8
1	B	503	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	163	VAL	2.8
1	B	488	TYR	2.8
1	B	374	GLN	2.7
1	B	278	GLY	2.7
1	B	35	PHE	2.7
1	B	259	ALA	2.7
1	B	549	ILE	2.6
1	B	161	ILE	2.5
1	B	162	PHE	2.5
1	B	433	ALA	2.5
1	B	253	GLY	2.5
1	B	15	VAL	2.5
1	B	233	TYR	2.5
1	B	227	PHE	2.4
1	B	438	CYS	2.4
1	B	489	TYR	2.4
1	B	115	ARG	2.4
1	B	42	GLN	2.4
1	B	504	VAL	2.4
1	B	32	ILE	2.3
1	B	60	ILE	2.3
1	B	129	PHE	2.3
1	B	31	GLY	2.3
1	B	216	ILE	2.3
1	B	67	GLY	2.2
1	B	40	PHE	2.2
1	B	300	ALA	2.2
1	B	56	TYR	2.2
1	B	224	ILE	2.2
1	B	284	ASP	2.2
1	B	185	SER	2.1
1	B	283	SER	2.1
1	B	276	GLU	2.1
1	B	157	GLY	2.0
1	B	136	PHE	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	PGE	A	1551	10/10	0.83	0.25	5.85	47,52,55,56	0
4	NAG	A	1553	14/15	0.90	0.17	2.49	44,56,60,62	0
4	NAG	A	1552	14/15	0.86	0.18	1.66	42,48,51,59	0
4	NAG	B	1551	14/15	0.81	0.21	1.03	75,81,85,85	0
2	7P9	B	1550	28/28	0.93	0.18	0.53	52,63,76,84	0
2	7P9	A	1550	28/28	0.93	0.15	0.36	39,51,62,66	0

6.5 Other polymers (i)

There are no such residues in this entry.