Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:33 AM GMT

PDB ID	:	3PBK
Title	:	Structural and Functional Studies of Fatty Acyl-Adenylate Ligases from E. coli and L. pneumophila
Authors	:	Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-10-20
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

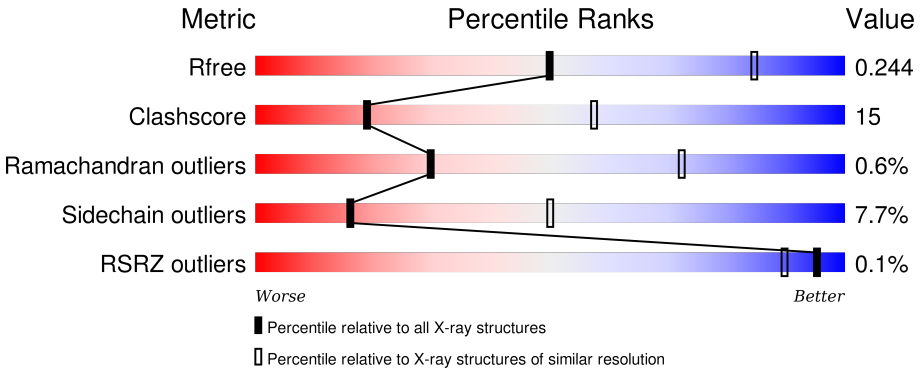
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	583	65% 27% • 5%
1	B	583	64% 26% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8732 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.

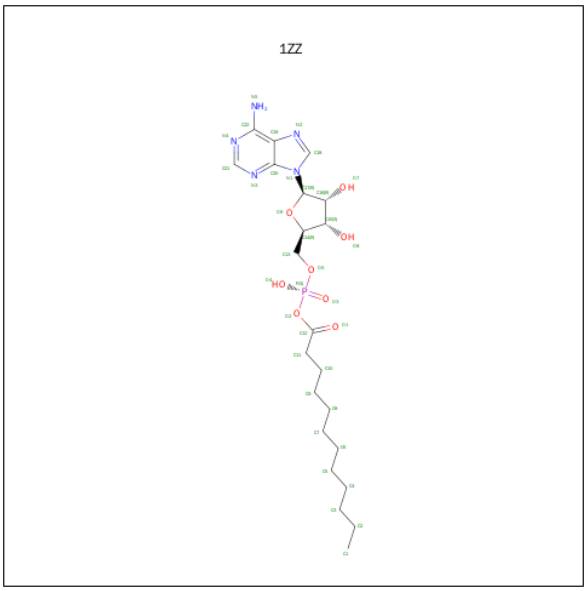
- Molecule 1 is a protein called Fatty Acyl-Adenylate Ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	Se	0	0	0
			4303	2729	750	804	11	9			
1	B	550	Total	C	N	O	S	Se	0	0	0
			4270	2713	744	794	11	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	EXPRESSION TAG	UNP Q8FDN4
A	3	SER	-	EXPRESSION TAG	UNP Q8FDN4
A	4	LEU	-	EXPRESSION TAG	UNP Q8FDN4
A	577	GLU	-	EXPRESSION TAG	UNP Q8FDN4
A	578	GLY	-	EXPRESSION TAG	UNP Q8FDN4
A	579	HIS	-	EXPRESSION TAG	UNP Q8FDN4
A	580	HIS	-	EXPRESSION TAG	UNP Q8FDN4
A	581	HIS	-	EXPRESSION TAG	UNP Q8FDN4
A	582	HIS	-	EXPRESSION TAG	UNP Q8FDN4
A	583	HIS	-	EXPRESSION TAG	UNP Q8FDN4
A	584	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	2	MSE	-	EXPRESSION TAG	UNP Q8FDN4
B	3	SER	-	EXPRESSION TAG	UNP Q8FDN4
B	4	LEU	-	EXPRESSION TAG	UNP Q8FDN4
B	577	GLU	-	EXPRESSION TAG	UNP Q8FDN4
B	578	GLY	-	EXPRESSION TAG	UNP Q8FDN4
B	579	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	580	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	581	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	582	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	583	HIS	-	EXPRESSION TAG	UNP Q8FDN4
B	584	HIS	-	EXPRESSION TAG	UNP Q8FDN4

- Molecule 2 is 5'-O-[(S)-(DODECANOYLOXY)(HYDROXY)PHOSPHORYL]ADENOSINE (three-letter code: 1ZZ) (formula: $C_{22}H_{36}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	22	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			36	22	5	8	1		

- Molecule 3 is water.

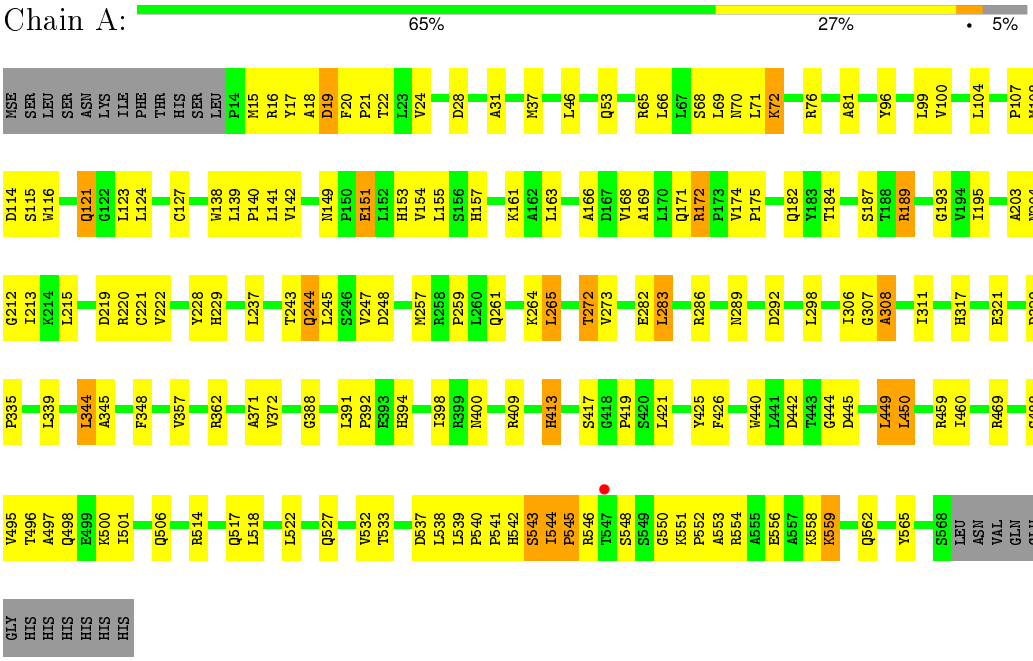
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	34	Total	O	0	0
			34	34		

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.

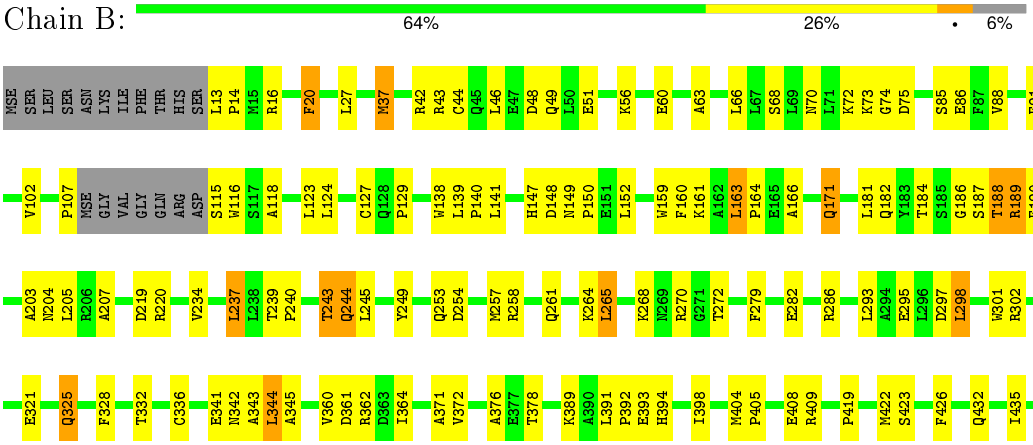
- Molecule 1: Fatty Acyl-Adenylate Ligase

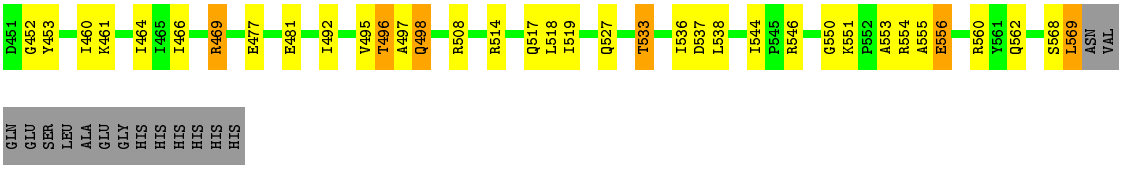
Chain A:



- Molecule 1: Fatty Acyl-Adenylate Ligase

Chain B:




D451
G452
Y453
I460
K461
I464
T465
I466
R469
E477
E481
I492
V495
T496
A497
Q498
R508
R514
Q517
L518
I519
Q527
T533
I536
D537
L538
I544
P545
R546
G550
K551
P552
A553
R554
A555
E556
R560
Y561
Q562
S568
L569
ASN
VAL
GLN
GLU
SER
LEU
ALA
GLU
GLY
HIS
HIS
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HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.47Å 118.34Å 137.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.82 – 3.00 89.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (89.82-3.00) 99.7 (89.82-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.190 , 0.251 0.189 , 0.244	Depositor DCC
R_{free} test set	1558 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 46619 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8732	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: 1ZZ

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	0.40	0/4389	0.55	0/5948
1	B	0.40	0/4356	0.54	0/5906
All	All	0.40	0/8745	0.54	0/11854

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	4303	0	4257	141	0
1	B	4270	0	4235	122	0
2	A	36	0	34	4	0
2	B	36	0	33	10	0
3	A	53	0	0	1	0
3	B	34	0	0	3	0
All	All	8732	0	8559	263	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 15.

All (263) 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:A:243:THR:HG22	1:A:245:LEU:HG	1.37	1.05
1:A:16:ARG:HH21	1:A:19:ASP:HB3	1.20	1.03
1:A:259:PRO:HG3	1:A:283:LEU:HD13	1.39	1.02
1:B:219:ASP:OD1	1:B:272:THR:HG21	1.62	0.99
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.23	0.99
1:B:445:ASP:OD1	2:B:585:1ZZ:O7	1.86	0.94
1:B:243:THR:HG23	1:B:245:LEU:HG	1.48	0.94
1:A:540:PRO:O	1:A:543:SER:HB3	1.69	0.92
1:A:497:ALA:H	1:A:562:GLN:HE22	1.17	0.92
1:A:204:ASN:HD21	1:A:345:ALA:H	1.16	0.92
1:A:553:ALA:HB1	1:A:556:GLU:HB3	1.54	0.90
1:A:219:ASP:OD1	1:A:272:THR:HG21	1.72	0.90
1:B:261:GLN:HE22	1:B:264:LYS:HE2	1.37	0.89
1:A:172:ARG:HG2	1:A:172:ARG:HH11	1.40	0.87
1:A:15:MSE:HE3	1:A:243:THR:HG23	1.56	0.85
1:A:272:THR:HG22	1:A:273:VAL:HG23	1.59	0.83
1:B:16:ARG:H	1:B:244:GLN:HE22	1.25	0.81
1:A:189:ARG:HH11	1:A:189:ARG:CG	1.93	0.81
1:A:496:THR:HG22	1:A:500:LYS:H	1.43	0.80
1:A:334:MSE:HE3	1:A:348:PHE:HD2	1.50	0.76
1:B:336:CYS:O	2:B:585:1ZZ:N5	2.19	0.76
1:B:466:ILE:HD11	1:B:469:ARG:HD2	1.68	0.76
1:A:496:THR:HG23	1:A:498:GLN:H	1.51	0.75
1:B:187:SER:O	1:B:188:THR:HB	1.86	0.74
1:A:172:ARG:CG	1:A:172:ARG:HH11	2.02	0.73
1:A:15:MSE:HA	1:A:244:GLN:HE22	1.52	0.73
1:B:186:GLY:HA3	1:B:191:PRO:HA	1.69	0.73
1:B:204:ASN:HD21	1:B:345:ALA:H	1.35	0.72
1:B:344:LEU:CD2	2:B:585:1ZZ:H10	2.20	0.71
1:A:501:ILE:HD12	1:A:532:VAL:HG21	1.72	0.71
1:B:544:ILE:HD13	1:B:560:ARG:HH12	1.55	0.71
1:A:344:LEU:HD22	2:A:1:1ZZ:H8	1.70	0.71
1:B:398:ILE:HG12	1:B:449:LEU:HD22	1.72	0.70
1:B:321:GLU:OE1	1:B:321:GLU:HA	1.91	0.70
1:B:13:LEU:HD12	1:B:14:PRO:HD2	1.72	0.70
1:B:422:MSE:HE3	1:B:435:ILE:HD11	1.74	0.69
1:A:16:ARG:HH21	1:A:19:ASP:CB	2.02	0.69
1:A:203:ALA:HB1	1:A:419:PRO:HB2	1.75	0.68
1:A:189:ARG:HG3	1:A:189:ARG:NH1	1.95	0.67
1:B:464:ILE:HG23	1:B:495:VAL:HB	1.77	0.67
1:A:16:ARG:NH2	1:A:19:ASP:HB3	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:CG2	1:B:245:LEU:HG	2.22	0.67
1:A:497:ALA:N	1:A:562:GLN:HE22	1.92	0.67
1:A:28:ASP:OD2	1:A:172:ARG:NH2	2.28	0.66
1:A:243:THR:CG2	1:A:245:LEU:HG	2.21	0.65
1:B:220:ARG:H	1:B:272:THR:HB	1.62	0.65
1:A:495:VAL:O	1:A:558:LYS:HE3	1.96	0.65
1:B:261:GLN:NE2	1:B:264:LYS:HE2	2.11	0.64
1:B:301:TRP:O	1:B:332:THR:HG21	1.97	0.64
1:A:221:CYS:HB2	1:A:247:VAL:HG23	1.80	0.64
1:B:308:ALA:O	1:B:551:LYS:HE3	1.99	0.63
1:A:182:GLN:NE2	1:A:184:THR:HG23	2.14	0.63
1:A:213:ILE:HD13	1:A:334:MSE:HE1	1.81	0.63
1:B:148:ASP:C	1:B:150:PRO:HD3	2.19	0.62
1:B:360:VAL:HG11	1:B:371:ALA:HB1	1.81	0.62
1:B:344:LEU:HD22	2:B:585:1ZZ:H10	1.81	0.62
1:B:37:MSE:HE1	1:B:237:LEU:HD23	1.81	0.62
1:A:207:ALA:HB1	1:A:391:LEU:HD13	1.80	0.62
1:A:546:ARG:HB3	1:A:551:LYS:O	2.00	0.62
1:A:398:ILE:HG12	1:A:449:LEU:HD22	1.81	0.61
1:B:115:SER:O	1:B:118:ALA:HB3	1.99	0.61
1:A:68:SER:CA	1:A:166:ALA:HB2	2.30	0.61
1:B:234:VAL:HG11	1:B:344:LEU:HB2	1.80	0.61
1:A:394:HIS:CE1	1:A:419:PRO:HD2	2.35	0.61
1:A:306:ILE:HD11	1:A:333:PHE:CD1	2.36	0.61
1:B:408:GLU:O	1:B:409:ARG:HB2	2.01	0.60
1:B:43:ARG:O	1:B:44:CYS:HB2	2.01	0.60
1:B:394:HIS:CE1	1:B:419:PRO:HD2	2.36	0.60
1:A:362:ARG:HH11	1:A:362:ARG:HG2	1.67	0.59
1:A:157:HIS:O	1:A:161:LYS:HG3	2.02	0.59
1:B:182:GLN:NE2	1:B:184:THR:HG23	2.17	0.59
1:B:72:LYS:O	1:B:75:ASP:HB2	2.02	0.59
1:B:107:PRO:HA	1:B:116:TRP:CD1	2.38	0.59
1:B:270:ARG:NH2	1:B:297:ASP:O	2.35	0.59
1:A:307:GLY:O	1:A:308:ALA:HB3	2.03	0.59
1:B:527:GLN:HE21	1:B:533:THR:CG2	2.16	0.59
1:A:172:ARG:NH1	1:A:172:ARG:CG	2.64	0.59
1:B:519:ILE:HG23	1:B:536:ILE:HB	1.84	0.58
1:B:207:ALA:HB1	1:B:391:LEU:HD22	1.85	0.58
1:A:544:ILE:O	1:A:545:PRO:O	2.21	0.58
1:A:344:LEU:CD2	2:A:1:1ZZ:H8	2.33	0.58
1:A:492:ILE:HG23	1:A:554:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:HB3	1:A:206:ARG:HA	1.85	0.57
1:A:261:GLN:NE2	1:A:264:LYS:HG3	2.19	0.57
1:B:508:ARG:HG3	1:B:508:ARG:O	2.05	0.57
1:B:302:ARG:O	1:B:332:THR:HG22	2.03	0.57
1:B:544:ILE:HD13	1:B:560:ARG:NH1	2.21	0.56
1:B:341:GLU:O	1:B:422:MSE:HG2	2.05	0.56
1:B:497:ALA:H	1:B:562:GLN:HE22	1.52	0.56
1:B:568:SER:O	1:B:569:LEU:HB2	2.05	0.56
1:A:334:MSE:HE3	1:A:348:PHE:CD2	2.38	0.56
1:A:153:HIS:HB3	1:A:155:LEU:HD11	1.88	0.56
1:B:127:CYS:SG	1:B:129:PRO:HD3	2.45	0.56
1:B:544:ILE:HD11	1:B:553:ALA:HB3	1.87	0.56
1:B:37:MSE:SE	1:B:88:VAL:HG11	2.56	0.55
1:B:527:GLN:HG2	1:B:533:THR:HG22	1.87	0.55
1:A:22:THR:HG22	1:A:24:VAL:H	1.72	0.55
1:B:445:ASP:CG	2:B:585:1ZZ:O7	2.46	0.54
1:B:392:PRO:O	1:B:393:GLU:HB2	2.06	0.54
1:A:551:LYS:HB2	1:A:552:PRO:CD	2.38	0.54
1:A:203:ALA:CB	1:A:419:PRO:HB2	2.37	0.54
1:A:15:MSE:HE3	1:A:243:THR:CG2	2.34	0.53
1:B:68:SER:HB3	1:B:166:ALA:HB2	1.89	0.53
1:B:389:LYS:HG3	1:B:453:TYR:CE1	2.43	0.53
1:A:76:ARG:HD2	1:A:127:CYS:HB2	1.90	0.52
1:A:222:VAL:HG13	1:A:265:LEU:HD12	1.90	0.52
1:A:496:THR:HG23	1:A:498:GLN:N	2.22	0.52
1:A:139:LEU:HB3	1:A:140:PRO:HD3	1.91	0.52
1:B:409:ARG:NH1	1:B:450:LEU:HD21	2.24	0.52
1:A:22:THR:HG22	1:A:24:VAL:N	2.24	0.52
1:B:362:ARG:HD3	3:B:610:HOH:O	2.10	0.52
1:A:459:ARG:HH11	1:A:551:LYS:HZ2	1.57	0.52
1:B:546:ARG:HD3	1:B:550:GLY:O	2.10	0.52
1:B:139:LEU:HB3	1:B:140:PRO:HD3	1.91	0.51
1:A:357:VAL:HG22	3:A:590:HOH:O	2.09	0.51
1:A:212:GLY:HA3	1:A:348:PHE:CD1	2.46	0.51
1:A:248:ASP:CB	1:A:265:LEU:HD11	2.40	0.51
1:A:544:ILE:N	1:A:545:PRO:HD3	2.26	0.51
1:A:138:TRP:O	1:A:142:VAL:HG23	2.10	0.51
1:A:107:PRO:HA	1:A:116:TRP:CD1	2.46	0.50
1:A:514:ARG:NH1	1:A:518:LEU:HB2	2.24	0.50
1:A:68:SER:N	1:A:166:ALA:HB2	2.26	0.50
1:A:237:LEU:C	1:A:237:LEU:HD23	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ILE:N	1:A:545:PRO:CD	2.75	0.50
1:B:477:GLU:O	1:B:481:GLU:HG3	2.10	0.50
1:A:195:ILE:HD11	1:A:426:PHE:HA	1.94	0.50
1:A:307:GLY:O	1:A:308:ALA:CB	2.60	0.50
1:B:477:GLU:OE1	1:B:554:ARG:NH2	2.42	0.50
1:B:42:ARG:HD2	1:B:258:ARG:HE	1.76	0.50
1:B:148:ASP:O	1:B:150:PRO:HD3	2.12	0.50
1:A:15:MSE:HA	1:A:244:GLN:NE2	2.22	0.49
1:B:422:MSE:HE3	1:B:435:ILE:CD1	2.42	0.49
1:A:496:THR:HG22	1:A:500:LYS:N	2.19	0.49
1:A:527:GLN:HG3	1:A:533:THR:HG22	1.94	0.49
1:B:239:THR:O	1:B:243:THR:HB	2.12	0.49
1:B:190:PHE:CZ	1:B:192:ARG:HD3	2.47	0.49
1:A:282:GLU:OE2	1:A:286:ARG:HD3	2.13	0.49
1:A:339:LEU:N	1:A:339:LEU:HD23	2.27	0.49
1:A:339:LEU:HA	2:A:1:1ZZ:H13A	1.94	0.49
1:A:398:ILE:HG12	1:A:449:LEU:CD2	2.43	0.49
1:A:243:THR:O	1:A:243:THR:HG22	2.13	0.48
1:A:444:GLY:O	1:A:460:ILE:HG13	2.12	0.48
1:B:186:GLY:CA	1:B:191:PRO:HA	2.42	0.48
1:B:461:LYS:HG2	1:B:555:ALA:HB2	1.96	0.48
1:B:48:ASP:OD1	1:B:49:GLN:N	2.46	0.48
1:A:445:ASP:OD1	2:A:1:1ZZ:O7	2.31	0.48
1:A:107:PRO:HD2	1:A:138:TRP:CZ3	2.48	0.48
1:A:72:LYS:HD2	1:A:72:LYS:N	2.29	0.48
1:B:342:ASN:O	1:B:343:ALA:HB3	2.14	0.48
1:A:413:HIS:HD2	1:A:442:ASP:OD2	1.96	0.48
1:B:311:ILE:HD12	3:B:609:HOH:O	2.14	0.48
1:B:307:GLY:O	1:B:308:ALA:HB3	2.14	0.48
1:A:123:LEU:HD13	1:A:123:LEU:O	2.14	0.48
1:A:154:VAL:C	1:A:155:LEU:HD12	2.35	0.47
1:B:496:THR:HG21	1:B:498:GLN:NE2	2.29	0.47
1:B:171:GLN:H	1:B:171:GLN:HG3	1.42	0.47
1:B:527:GLN:HE21	1:B:533:THR:HG22	1.79	0.47
1:A:248:ASP:HB2	1:A:265:LEU:HD11	1.96	0.47
1:B:257:MSE:HA	1:B:257:MSE:HE3	1.97	0.47
1:A:219:ASP:CG	1:A:272:THR:HG21	2.35	0.47
1:A:213:ILE:HD13	1:A:334:MSE:CE	2.44	0.47
1:A:68:SER:HA	1:A:166:ALA:HB2	1.96	0.47
1:A:153:HIS:HB3	1:A:155:LEU:CD1	2.44	0.47
1:B:508:ARG:CG	1:B:508:ARG:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD11	1:A:155:LEU:HD21	1.95	0.47
1:B:336:CYS:SG	2:B:585:1ZZ:H8A	2.55	0.47
1:A:398:ILE:CG1	1:A:449:LEU:HD22	2.43	0.46
1:B:492:ILE:HG23	1:B:554:ARG:HG2	1.97	0.46
1:B:56:LYS:O	1:B:60:GLU:HG3	2.15	0.46
1:B:239:THR:HB	1:B:240:PRO:HD3	1.96	0.46
1:B:344:LEU:HD22	2:B:585:1ZZ:C7	2.46	0.46
1:A:24:VAL:HG22	1:A:96:TYR:CD1	2.51	0.46
1:B:149:ASN:O	1:B:152:LEU:HB3	2.16	0.46
1:A:168:VAL:HG22	1:A:169:ALA:N	2.31	0.46
1:A:459:ARG:HD2	1:A:551:LYS:NZ	2.31	0.46
1:B:203:ALA:HB1	1:B:419:PRO:HB2	1.97	0.46
1:B:66:LEU:HG	1:B:160:PHE:HE1	1.80	0.46
1:A:539:LEU:HB3	1:A:540:PRO:CD	2.45	0.46
1:B:60:GLU:O	1:B:63:ALA:HB3	2.16	0.46
1:B:91:PHE:O	1:B:94:CYS:HB2	2.16	0.46
1:B:43:ARG:HB2	1:B:43:ARG:CZ	2.46	0.45
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.81	0.45
1:B:497:ALA:H	1:B:562:GLN:NE2	2.13	0.45
1:A:66:LEU:HD13	1:A:99:LEU:HD12	1.97	0.45
1:A:518:LEU:O	1:A:522:LEU:HB2	2.16	0.45
1:B:344:LEU:HD13	2:B:585:1ZZ:H5A	1.97	0.45
1:B:73:LYS:HG3	1:B:74:GLY:N	2.31	0.45
1:A:149:ASN:HB3	1:A:151:GLU:OE1	2.17	0.45
1:A:541:PRO:HA	1:A:542:HIS:HA	1.68	0.45
1:A:362:ARG:HG2	1:A:362:ARG:NH1	2.29	0.45
1:A:348:PHE:O	1:A:388:GLY:HA3	2.17	0.45
1:A:289:ASN:O	1:A:292:ASP:HB2	2.16	0.45
1:A:334:MSE:CE	1:A:348:PHE:HD2	2.26	0.44
1:B:279:PHE:CD1	1:B:279:PHE:C	2.91	0.44
1:B:234:VAL:HG12	1:B:344:LEU:HD12	1.99	0.44
1:B:116:TRP:CZ3	1:B:141:LEU:HD22	2.51	0.44
1:A:229:HIS:CE1	1:A:550:GLY:HA3	2.52	0.44
1:A:155:LEU:N	1:A:155:LEU:HD12	2.32	0.44
1:A:311:ILE:HD13	1:A:335:PRO:HB3	2.00	0.44
1:A:220:ARG:H	1:A:272:THR:HB	1.82	0.44
1:B:298:LEU:HD23	1:B:328:PHE:HB2	2.00	0.44
1:A:329:ASP:HB3	1:A:332:THR:HG23	2.00	0.44
1:A:31:ALA:HB1	1:A:53:GLN:HA	1.99	0.43
1:B:189:ARG:HD3	1:B:189:ARG:HA	1.72	0.43
1:A:546:ARG:NH2	1:A:552:PRO:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:OE2	1:B:286:ARG:HD3	2.17	0.43
1:B:376:ALA:C	1:B:378:THR:H	2.21	0.43
1:B:37:MSE:HE2	1:B:249:TYR:OH	2.18	0.43
1:A:112:GLN:O	1:A:115:SER:HB3	2.18	0.43
1:A:506:GLN:HG3	1:A:506:GLN:O	2.18	0.43
1:A:121:GLN:HE21	1:A:121:GLN:HB3	1.56	0.43
1:B:68:SER:CB	1:B:166:ALA:HB2	2.48	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.64	0.43
1:A:20:PHE:HA	1:A:21:PRO:HD3	1.79	0.43
1:A:317:HIS:CD2	1:A:321:GLU:HG2	2.54	0.43
1:A:371:ALA:O	1:A:409:ARG:HB3	2.19	0.43
1:B:362:ARG:HH11	1:B:362:ARG:HG2	1.84	0.43
1:A:215:LEU:HD13	1:A:243:THR:HG21	2.01	0.42
1:B:466:ILE:HG12	1:B:469:ARG:O	2.19	0.42
1:A:66:LEU:O	1:A:71:LEU:HD12	2.18	0.42
1:B:195:ILE:HD11	1:B:426:PHE:HA	1.99	0.42
1:A:559:LYS:N	1:A:559:LYS:HD2	2.34	0.42
1:B:163:LEU:HA	1:B:164:PRO:HD3	1.77	0.42
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.34	0.42
1:A:189:ARG:HA	1:A:189:ARG:HD2	1.86	0.42
1:A:442:ASP:C	1:A:442:ASP:OD1	2.57	0.42
1:B:51:GLU:HG3	3:B:591:HOH:O	2.19	0.42
1:A:237:LEU:O	1:A:237:LEU:HD23	2.19	0.42
1:B:27:LEU:HD23	1:B:96:TYR:CE1	2.54	0.42
1:A:107:PRO:C	1:A:109:GLY:H	2.23	0.42
1:B:308:ALA:HA	2:B:585:1ZZ:O1	2.20	0.42
1:A:22:THR:CG2	1:A:24:VAL:H	2.33	0.42
1:B:159:TRP:O	1:B:163:LEU:HD13	2.20	0.42
1:B:514:ARG:CZ	1:B:518:LEU:HD12	2.50	0.42
1:A:392:PRO:O	1:A:394:HIS:HD2	2.02	0.41
1:B:293:LEU:HD13	1:B:325:GLN:OE1	2.21	0.41
1:B:86:GLU:HG2	1:B:161:LYS:NZ	2.35	0.41
1:B:423:SER:O	1:B:432:GLN:HA	2.20	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD12	1.82	0.41
1:B:102:VAL:HG22	1:B:181:LEU:HB2	2.02	0.41
1:A:417:SER:HB3	1:A:440:TRP:CE3	2.55	0.41
1:A:204:ASN:ND2	1:A:345:ALA:H	1.98	0.41
1:B:107:PRO:HG2	1:B:138:TRP:CE3	2.56	0.41
1:B:20:PHE:N	1:B:20:PHE:CD2	2.87	0.41
1:B:389:LYS:HG2	1:B:452:GLY:O	2.21	0.41
1:A:76:ARG:HG3	1:A:100:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.79	0.41
1:A:15:MSE:HE2	1:A:17:TYR:CZ	2.55	0.41
1:B:344:LEU:HD22	2:B:585:1ZZ:H7	2.03	0.41
1:A:494:PHE:CE2	1:A:558:LYS:HA	2.56	0.41
1:B:253:GLN:HG2	1:B:254:ASP:N	2.36	0.41
1:A:24:VAL:HG22	1:A:96:TYR:CE1	2.56	0.41
1:A:400:ASN:C	1:A:400:ASN:OD1	2.59	0.40
1:A:81:ALA:HB3	1:A:228:TYR:HB3	2.03	0.40
1:A:174:VAL:HG23	1:A:175:PRO:N	2.35	0.40
1:B:404:MSE:HE3	1:B:405:PRO:HD2	2.02	0.40
1:B:188:THR:HG23	1:B:189:ARG:N	2.36	0.40
1:A:104:LEU:CD2	1:A:123:LEU:HG	2.51	0.40
1:A:193:GLY:O	1:A:425:TYR:HA	2.21	0.40
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.86	0.40
1:B:361:ASP:HB3	1:B:364:ILE:HD12	2.03	0.40
1:B:556:GLU:HG2	1:B:560:ARG:NH2	2.37	0.40
1:B:325:GLN:HE21	1:B:325:GLN:HB3	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/583 (95%)	522 (94%)	27 (5%)	4 (1%)	26	70
1	B	546/583 (94%)	512 (94%)	31 (6%)	3 (0%)	34	76
All	All	1099/1166 (94%)	1034 (94%)	58 (5%)	7 (1%)	30	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP

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Mol	Chain	Res	Type
1	A	545	PRO
1	B	147	HIS
1	A	308	ALA
1	B	188	THR
1	B	308	ALA
1	A	544	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/467 (96%)	414 (92%)	36 (8%)	15	47
1	B	447/467 (96%)	414 (93%)	33 (7%)	17	52
All	All	897/934 (96%)	828 (92%)	69 (8%)	16	50

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	MSE
1	A	46	LEU
1	A	70	ASN
1	A	72	LYS
1	A	108	MSE
1	A	114	ASP
1	A	121	GLN
1	A	124	LEU
1	A	151	GLU
1	A	163	LEU
1	A	171	GLN
1	A	172	ARG
1	A	187	SER
1	A	189	ARG
1	A	205	LEU
1	A	244	GLN
1	A	257	MSE

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Mol	Chain	Res	Type
1	A	265	LEU
1	A	272	THR
1	A	283	LEU
1	A	298	LEU
1	A	344	LEU
1	A	372	VAL
1	A	413	HIS
1	A	421	LEU
1	A	449	LEU
1	A	450	LEU
1	A	469	ARG
1	A	488	SER
1	A	517	GLN
1	A	537	ASP
1	A	538	LEU
1	A	543	SER
1	A	548	SER
1	A	559	LYS
1	A	565	TYR
1	B	20	PHE
1	B	37	MSE
1	B	46	LEU
1	B	70	ASN
1	B	85	SER
1	B	123	LEU
1	B	124	LEU
1	B	163	LEU
1	B	171	GLN
1	B	189	ARG
1	B	205	LEU
1	B	237	LEU
1	B	243	THR
1	B	244	GLN
1	B	265	LEU
1	B	268	LYS
1	B	295	GLU
1	B	298	LEU
1	B	325	GLN
1	B	344	LEU
1	B	372	VAL
1	B	449	LEU
1	B	450	LEU

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Mol	Chain	Res	Type
1	B	460	ILE
1	B	469	ARG
1	B	496	THR
1	B	498	GLN
1	B	517	GLN
1	B	533	THR
1	B	537	ASP
1	B	538	LEU
1	B	556	GLU
1	B	569	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	95	GLN
1	A	121	GLN
1	A	143	ASN
1	A	157	HIS
1	A	176	ASN
1	A	182	GLN
1	A	204	ASN
1	A	229	HIS
1	A	244	GLN
1	A	261	GLN
1	A	269	ASN
1	A	342	ASN
1	A	394	HIS
1	A	413	HIS
1	A	517	GLN
1	A	562	GLN
1	B	95	GLN
1	B	182	GLN
1	B	204	ASN
1	B	244	GLN
1	B	261	GLN
1	B	269	ASN
1	B	315	GLN
1	B	318	GLN
1	B	342	ASN
1	B	394	HIS
1	B	517	GLN

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Mol	Chain	Res	Type
1	B	527	GLN
1	B	562	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1ZZ	A	1	-	32,38,38	1.57	8 (25%)	34,52,52	2.64	11 (32%)
2	1ZZ	B	585	-	32,38,38	1.78	9 (28%)	34,52,52	2.92	12 (35%)

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	1ZZ	A	1	-	-	0/20/42/42	0/3/3/3
2	1ZZ	B	585	-	-	0/20/42/42	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	585	1ZZ	P-O4	-4.21	1.37	1.54
2	B	585	1ZZ	C19-C20	-4.13	1.31	1.40
2	A	1	1ZZ	P-O4	-4.01	1.37	1.54
2	A	1	1ZZ	C19-C20	-4.00	1.31	1.40
2	B	585	1ZZ	C21-N4	-3.35	1.27	1.33
2	B	585	1ZZ	C15-C16	-2.52	1.46	1.53
2	A	1	1ZZ	C15-C16	-2.16	1.47	1.53
2	A	1	1ZZ	C22-N5	2.07	1.41	1.34
2	A	1	1ZZ	C20-N3	2.14	1.38	1.35
2	A	1	1ZZ	C21-N3	2.23	1.36	1.32
2	A	1	1ZZ	P-O3	2.28	1.59	1.51
2	A	1	1ZZ	P-O2	2.31	1.65	1.60
2	B	585	1ZZ	C18-N2	2.37	1.39	1.34
2	B	585	1ZZ	P-O3	2.37	1.59	1.51
2	B	585	1ZZ	P-O2	2.83	1.66	1.60
2	B	585	1ZZ	C22-N5	2.89	1.43	1.34
2	B	585	1ZZ	C20-N3	2.96	1.40	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	585	1ZZ	N3-C21-N4	-12.91	119.01	128.89
2	A	1	1ZZ	N3-C21-N4	-10.22	121.07	128.89
2	A	1	1ZZ	O6-C14-C15	-4.40	96.29	105.15
2	A	1	1ZZ	O1-C12-C11	-3.72	108.83	123.72
2	B	585	1ZZ	O6-C17-N1	-3.09	101.63	108.10
2	A	1	1ZZ	O6-C17-N1	-2.32	103.23	108.10
2	B	585	1ZZ	O4-P-O3	-2.01	101.65	112.53
2	B	585	1ZZ	C9-C10-C11	2.14	121.13	113.29
2	A	1	1ZZ	O4-P-O2	2.19	110.94	104.16
2	A	1	1ZZ	O5-C13-C14	2.26	117.46	109.12
2	B	585	1ZZ	O7-C16-C15	2.27	119.20	111.83
2	B	585	1ZZ	C17-N1-C20	2.50	130.71	126.94
2	A	1	1ZZ	C13-C14-C15	2.52	125.22	115.21
2	B	585	1ZZ	O6-C14-C13	2.57	118.50	109.32
2	A	1	1ZZ	O2-P-O3	2.77	117.51	108.38
2	B	585	1ZZ	C10-C11-C12	3.10	125.79	113.59
2	B	585	1ZZ	O5-C13-C14	3.11	120.58	109.12
2	B	585	1ZZ	O2-P-O3	3.19	118.90	108.38
2	A	1	1ZZ	O7-C16-C15	3.48	123.14	111.83
2	B	585	1ZZ	O8-C15-C14	3.60	121.85	111.05
2	A	1	1ZZ	C9-C10-C11	3.83	127.35	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	585	1ZZ	O2-P-O5	4.89	115.60	102.86
2	A	1	1ZZ	O8-C15-C14	4.93	125.83	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	1ZZ	4	0
2	B	585	1ZZ	10	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	546/583 (93%)	-0.59	1 (0%) 95 87	14, 24, 47, 66	0
1	B	542/583 (92%)	-0.66	0 100 100	15, 25, 48, 70	0
All	All	1088/1166 (93%)	-0.62	1 (0%) 95 90	14, 25, 48, 70	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	THR	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	1ZZ	B	585	36/36	0.95	0.18	0.71	16,19,22,23	0
2	1ZZ	A	1	36/36	0.94	0.21	0.42	15,21,25,28	0

6.5 Other polymers (i)

There are no such residues in this entry.