Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 05:43 pm BST

PDB ID	:	1MZO
Title	:	Crystal structure of pyruvate formate-lyase with pyruvate
Authors	:	Lehtio, L.; Leppanen, V.-M.; Kozarich, J.W.; Goldman, A.
Deposited on	:	2002-10-09
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (i)) 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	:	2.11
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)	:	2.11

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 2.70 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	Percentile Ranks	Value
Rfree		0.232
Clashscore		14
Ramachandran outliers		0.3%
Sidechain outliers		4.5%
RSRZ outliers		1.5%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
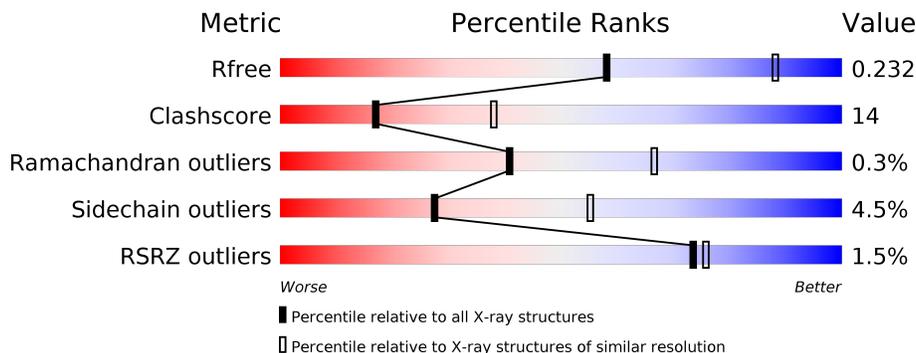
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	A	759	71% 26%
1	B	759	71% 27%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12467 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 Pyruvate formate-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			5965	3770	1020	1139	36			
1	B	756	Total	C	N	O	S	0	0	0
			5965	3770	1020	1139	36			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
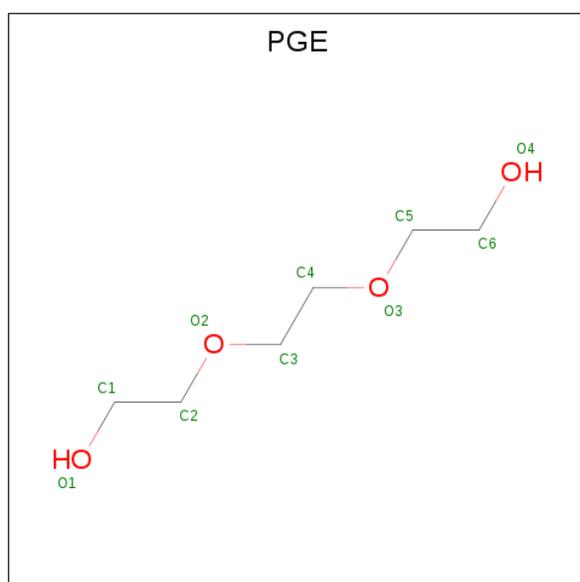
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).

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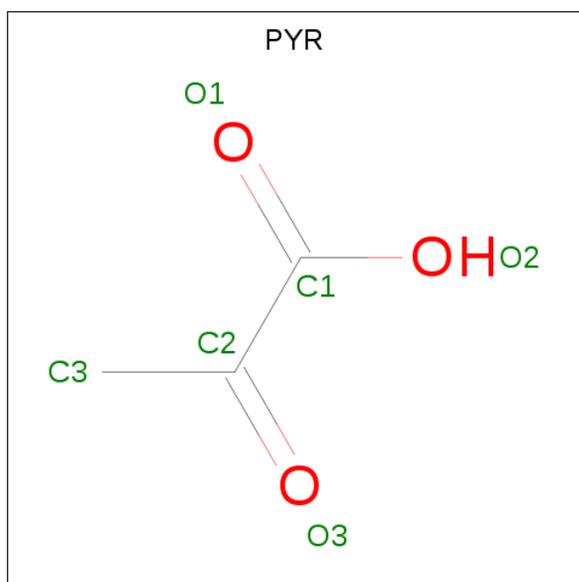
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	276	Total 276	O 276	0	0
4	B	239	Total 239	O 239	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Pyruvate formate-lyase
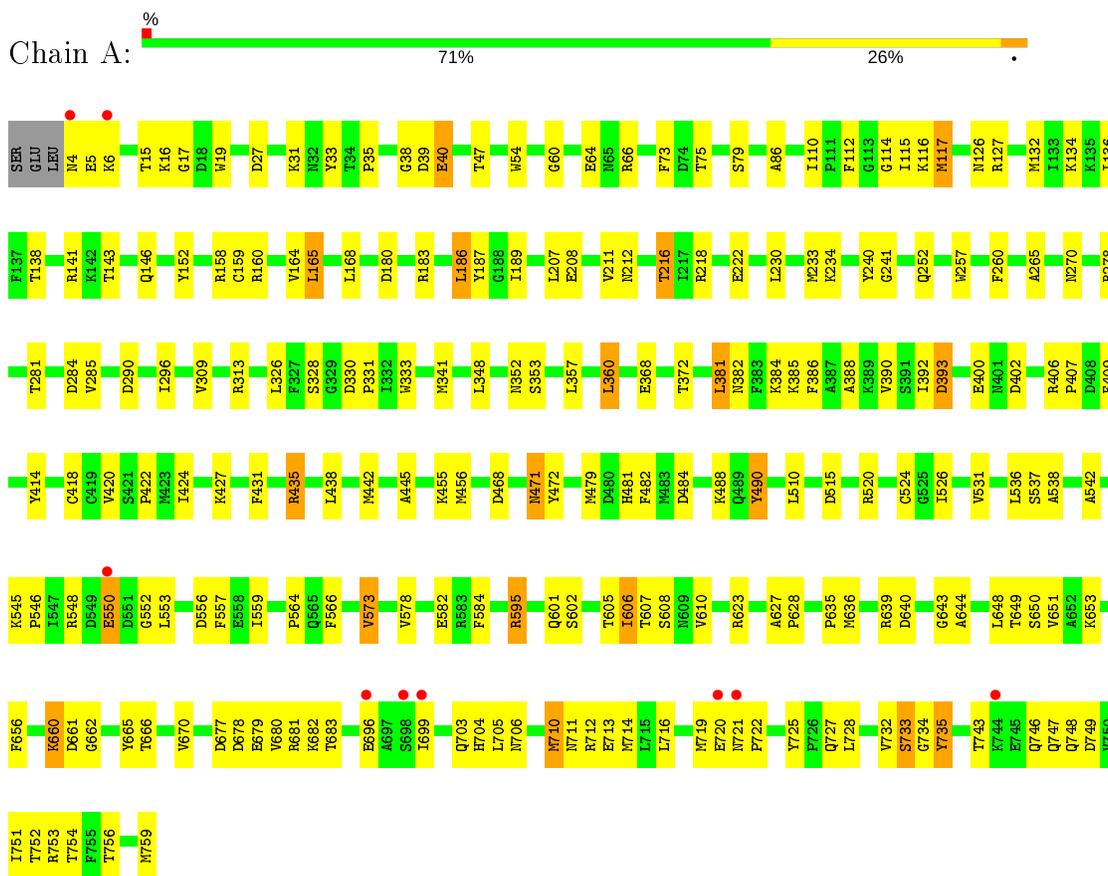
- Molecule 1: Pyruvate formate-lyase
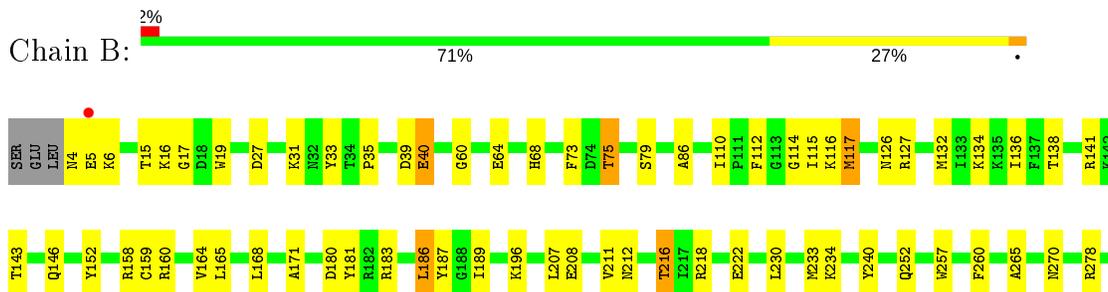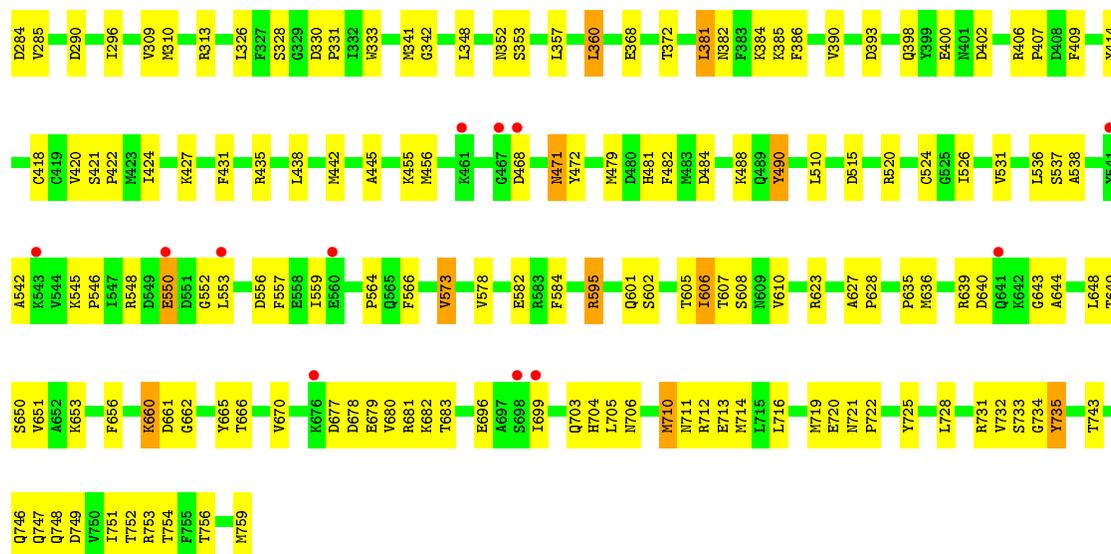
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	158.35Å 158.35Å 159.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.79 – 2.68	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 94.3 (19.79-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.235 0.192 , 0.232	Depositor DCC
R_{free} test set	2795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.004 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12467	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.37	0/6086	0.60	0/8222
1	B	0.38	0/6086	0.60	0/8222
All	All	0.37	0/12172	0.60	0/16444

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	Sidechain

5.2 Too-close contacts (i)

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	5965	0	5889	169	0
1	B	5965	0	5889	165	0
2	A	10	0	14	1	1
3	A	6	0	3	1	0
3	B	6	0	3	0	0
4	A	276	0	0	12	0
4	B	239	0	0	7	0
All	All	12467	0	11798	332	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 14.

All (332) 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:602:SER:HB3	1:A:661:ASP:HB3	1.43	1.00
1:B:602:SER:HB3	1:B:661:ASP:HB3	1.44	0.97
1:B:606:ILE:HG22	1:B:607:THR:H	1.41	0.85
1:A:606:ILE:HG22	1:A:607:THR:H	1.43	0.83
1:A:115:ILE:HG22	4:A:2049:HOH:O	1.77	0.82
1:A:112:PHE:HD1	4:A:2137:HOH:O	1.63	0.80
1:A:341:MET:HB2	1:A:406:ARG:NH1	1.97	0.79
1:B:4:ASN:ND2	1:B:6:LYS:HB2	2.00	0.77
1:A:4:ASN:ND2	1:A:6:LYS:HB2	2.00	0.76
1:B:341:MET:HB2	1:B:406:ARG:NH1	2.00	0.76
1:B:4:ASN:HD21	1:B:6:LYS:HB2	1.50	0.75
1:A:4:ASN:HD21	1:A:6:LYS:HB2	1.51	0.75
1:A:420:VAL:HG23	1:A:662:GLY:HA3	1.68	0.74
1:A:40:GLU:HG2	1:A:386:PHE:CD1	2.23	0.74
1:B:40:GLU:HG2	1:B:386:PHE:CD1	2.22	0.73
1:A:333:TRP:HE1	1:A:735:TYR:HB3	1.53	0.73
1:B:420:VAL:HG23	1:B:662:GLY:HA3	1.70	0.73
1:A:564:PRO:HB2	1:A:573:VAL:HG22	1.71	0.73
1:A:39:ASP:HB3	1:A:382:ASN:ND2	2.04	0.71
1:B:564:PRO:HB2	1:B:573:VAL:HG22	1.72	0.71
1:B:666:THR:HA	1:B:706:ASN:HB2	1.72	0.71
1:B:39:ASP:HB3	1:B:382:ASN:ND2	2.04	0.71
1:A:328:SER:HB3	1:A:746:GLN:NE2	2.04	0.71
1:B:333:TRP:HE1	1:B:735:TYR:HB3	1.56	0.70
1:B:328:SER:HB3	1:B:746:GLN:NE2	2.06	0.70
1:A:666:THR:HA	1:A:706:ASN:HB2	1.73	0.70
1:B:115:ILE:HG21	1:B:138:THR:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HD2	4:A:2200:HOH:O	1.92	0.68
1:B:720:GLU:C	1:B:722:PRO:HD3	2.13	0.68
1:A:720:GLU:C	1:A:722:PRO:HD3	2.14	0.68
1:A:115:ILE:HG21	1:A:138:THR:HG22	1.76	0.68
1:B:40:GLU:HG2	1:B:386:PHE:CG	2.28	0.67
1:B:212:ASN:O	1:B:216:THR:HG22	1.95	0.67
1:A:526:ILE:HD11	1:A:584:PHE:CD2	2.30	0.66
1:A:212:ASN:O	1:A:216:THR:HG22	1.95	0.66
1:A:40:GLU:HG2	1:A:386:PHE:CG	2.30	0.66
1:A:743:THR:OG1	1:A:746:GLN:HG3	1.96	0.66
1:B:526:ILE:HD11	1:B:584:PHE:CD2	2.31	0.65
1:B:696:GLU:HB2	1:B:699:ILE:CG2	2.26	0.65
1:A:696:GLU:HB2	1:A:699:ILE:CG2	2.27	0.65
1:B:743:THR:OG1	1:B:746:GLN:HG3	1.97	0.65
1:B:218:ARG:O	1:B:222:GLU:HG3	1.97	0.64
1:A:623:ARG:NH1	1:A:627:ALA:O	2.32	0.63
1:A:218:ARG:O	1:A:222:GLU:HG3	1.98	0.63
1:B:749:ASP:O	1:B:753:ARG:HG3	1.98	0.63
1:A:333:TRP:NE1	1:A:735:TYR:HB3	2.14	0.62
1:B:706:ASN:HD21	1:B:734:GLY:N	1.98	0.62
1:A:725:TYR:HB3	1:A:728:LEU:HB2	1.82	0.62
1:B:602:SER:HB3	1:B:661:ASP:CB	2.27	0.62
1:A:743:THR:O	1:A:747:GLN:HG3	1.99	0.62
1:B:623:ARG:NH1	1:B:627:ALA:O	2.33	0.61
1:A:605:THR:O	1:A:608:SER:HB2	2.00	0.61
1:B:725:TYR:HB3	1:B:728:LEU:HB2	1.82	0.61
1:B:696:GLU:HB2	1:B:699:ILE:HG23	1.82	0.61
1:A:696:GLU:HB2	1:A:699:ILE:HG23	1.82	0.61
1:A:656:PHE:O	1:A:660:LYS:HD2	2.00	0.61
1:A:706:ASN:HD21	1:A:734:GLY:N	1.99	0.61
1:A:749:ASP:O	1:A:753:ARG:HG3	2.01	0.61
1:B:333:TRP:NE1	1:B:735:TYR:HB3	2.16	0.61
1:A:420:VAL:CG2	1:A:662:GLY:HA3	2.31	0.60
1:B:743:THR:O	1:B:747:GLN:HG3	2.01	0.60
1:B:75:THR:HG21	4:B:2241:HOH:O	2.01	0.60
1:A:678:ASP:O	1:A:682:LYS:HG3	2.02	0.59
1:B:420:VAL:CG2	1:B:662:GLY:HA3	2.32	0.59
1:B:670:VAL:HG13	1:B:711:ASN:ND2	2.16	0.59
1:A:670:VAL:HG13	1:A:711:ASN:ND2	2.16	0.59
1:B:605:THR:O	1:B:608:SER:HB2	2.02	0.59
1:B:559:ILE:HD12	1:B:559:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:PHE:O	1:B:660:LYS:HD2	2.02	0.59
1:B:115:ILE:HG21	1:B:138:THR:CG2	2.33	0.59
1:B:644:ALA:HB2	1:B:756:THR:HG21	1.84	0.59
1:B:678:ASP:O	1:B:682:LYS:HG3	2.03	0.58
1:A:559:ILE:N	1:A:559:ILE:HD12	2.17	0.58
1:A:115:ILE:HG21	1:A:138:THR:CG2	2.34	0.58
1:B:39:ASP:HB3	1:B:382:ASN:HD22	1.68	0.58
1:A:15:THR:HB	1:A:31:LYS:O	2.04	0.58
1:B:606:ILE:HG22	1:B:607:THR:N	2.14	0.58
1:A:644:ALA:HB2	1:A:756:THR:HG21	1.85	0.58
1:A:39:ASP:HB3	1:A:382:ASN:HD22	1.68	0.58
1:B:548:ARG:HG3	1:B:548:ARG:HH11	1.69	0.58
1:B:15:THR:HB	1:B:31:LYS:O	2.04	0.58
1:B:566:PHE:O	1:B:635:PRO:HB3	2.04	0.58
1:B:278:ARG:HD2	4:B:2091:HOH:O	2.04	0.57
1:A:606:ILE:HG22	1:A:607:THR:N	2.16	0.56
1:A:431:PHE:CZ	1:A:520:ARG:HD3	2.40	0.56
1:B:402:ASP:OD2	1:B:406:ARG:NH1	2.38	0.56
1:A:110:ILE:HG13	1:A:270:ASN:HB3	1.87	0.56
1:A:341:MET:O	1:A:406:ARG:HD3	2.05	0.56
1:A:656:PHE:CD1	1:A:703:GLN:HG3	2.40	0.56
1:B:712:ARG:HH12	1:B:751:ILE:HB	1.70	0.56
1:B:431:PHE:CZ	1:B:520:ARG:HD3	2.41	0.56
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.71	0.56
1:B:110:ILE:HG13	1:B:270:ASN:HB3	1.87	0.56
1:A:402:ASP:OD2	1:A:406:ARG:NH1	2.40	0.55
1:B:341:MET:O	1:B:406:ARG:HD3	2.06	0.55
1:B:284:ASP:HB2	1:B:352:ASN:HB2	1.88	0.55
1:B:720:GLU:O	1:B:722:PRO:HD3	2.06	0.55
1:B:656:PHE:CD1	1:B:703:GLN:HG3	2.41	0.55
1:B:677:ASP:O	1:B:681:ARG:HG3	2.07	0.55
1:A:284:ASP:HB2	1:A:352:ASN:HB2	1.89	0.55
1:A:602:SER:HB3	1:A:661:ASP:CB	2.26	0.55
1:B:357:LEU:O	1:B:360:LEU:HB2	2.07	0.55
1:A:720:GLU:O	1:A:722:PRO:HD3	2.07	0.54
1:B:409:PHE:HE2	1:B:422:PRO:HB2	1.72	0.54
1:A:566:PHE:O	1:A:635:PRO:HB3	2.06	0.54
1:A:712:ARG:HH12	1:A:751:ILE:HB	1.72	0.54
1:A:677:ASP:O	1:A:681:ARG:HG3	2.07	0.54
1:B:595:ARG:HD3	4:B:2119:HOH:O	2.07	0.54
1:A:290:ASP:HB3	1:A:296:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASP:HB3	1:B:296:ILE:HG12	1.89	0.53
1:A:33:TYR:CE1	1:A:35:PRO:HG3	2.43	0.53
1:A:357:LEU:O	1:A:360:LEU:HB2	2.08	0.53
1:A:712:ARG:O	1:A:716:LEU:HD13	2.08	0.53
1:B:712:ARG:NH1	1:B:751:ILE:HB	2.24	0.53
1:A:488:LYS:HD2	1:B:208:GLU:O	2.09	0.53
1:A:189:ILE:HG21	1:A:234:LYS:HG3	1.91	0.53
1:B:651:VAL:HG11	1:B:665:TYR:HB2	1.90	0.53
1:B:712:ARG:O	1:B:716:LEU:HD13	2.08	0.53
1:A:409:PHE:HE2	1:A:422:PRO:HB2	1.73	0.52
1:A:418:CYS:SG	3:A:2001:PYR:C2	2.97	0.52
1:A:372:THR:HG21	1:A:400:GLU:HG3	1.90	0.52
1:A:330:ASP:N	1:A:331:PRO:CD	2.73	0.52
1:B:372:THR:HG21	1:B:400:GLU:HG3	1.91	0.52
1:B:189:ILE:HG21	1:B:234:LYS:HG3	1.92	0.52
1:B:330:ASP:N	1:B:331:PRO:CD	2.73	0.52
1:A:385:LYS:NZ	1:A:683:THR:HG22	2.25	0.52
1:B:132:MET:HE3	1:B:136:ILE:HG13	1.92	0.52
1:A:180:ASP:HB3	1:A:183:ARG:HG3	1.91	0.51
1:A:165:LEU:HD11	1:A:490:TYR:HA	1.92	0.51
1:A:651:VAL:HG11	1:A:665:TYR:HB2	1.91	0.51
1:B:165:LEU:HD11	1:B:490:TYR:HA	1.92	0.51
1:A:550:GLU:HA	1:A:550:GLU:OE1	2.11	0.51
1:A:677:ASP:OD2	1:A:679:GLU:HB2	2.11	0.51
1:A:208:GLU:O	1:B:488:LYS:HD2	2.10	0.51
1:B:704:HIS:CG	1:B:705:LEU:N	2.79	0.51
1:B:385:LYS:NZ	1:B:683:THR:HG22	2.26	0.51
1:A:704:HIS:CG	1:A:705:LEU:N	2.79	0.51
1:B:677:ASP:OD2	1:B:679:GLU:HB2	2.11	0.51
1:B:643:GLY:HA3	1:B:759:MET:OXT	2.11	0.51
1:A:643:GLY:HA3	1:A:759:MET:OXT	2.12	0.50
1:A:146:GLN:HG2	4:A:2074:HOH:O	2.11	0.50
1:B:445:ALA:HA	1:B:482:PHE:CE2	2.46	0.50
1:A:116:LYS:HB2	1:A:117:MET:HE1	1.93	0.50
1:B:186:LEU:HD13	1:B:187:TYR:CE1	2.47	0.50
1:B:420:VAL:O	1:B:422:PRO:HD3	2.11	0.50
1:A:222:GLU:CD	1:A:595:ARG:HH22	2.15	0.50
1:A:712:ARG:NH1	1:A:751:ILE:HB	2.26	0.50
1:B:648:LEU:HD23	1:B:665:TYR:HE2	1.77	0.50
1:A:328:SER:CB	1:A:746:GLN:NE2	2.73	0.50
1:A:393:ASP:HA	4:A:2108:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:THR:O	1:A:653:LYS:HG3	2.12	0.49
1:A:445:ALA:HA	1:A:482:PHE:CE2	2.48	0.49
1:A:66:ARG:HD2	4:A:2207:HOH:O	2.12	0.49
1:B:649:THR:O	1:B:653:LYS:HG3	2.12	0.49
1:A:112:PHE:HE1	4:A:2141:HOH:O	1.95	0.49
1:A:420:VAL:O	1:A:422:PRO:HD3	2.12	0.49
1:B:158:ARG:HG2	1:B:456:MET:CE	2.42	0.49
1:B:132:MET:O	1:B:132:MET:HE3	2.11	0.49
1:A:471:ASN:HD22	1:A:472:TYR:N	2.11	0.49
1:B:132:MET:CE	1:B:136:ILE:HG13	2.43	0.49
1:A:222:GLU:OE2	1:A:595:ARG:NH2	2.46	0.49
1:B:116:LYS:HB2	1:B:117:MET:HE1	1.94	0.49
1:A:696:GLU:HB2	1:A:699:ILE:HG22	1.95	0.49
1:A:19:TRP:HD1	1:A:27:ASP:OD1	1.95	0.49
1:A:648:LEU:HD23	1:A:665:TYR:HE2	1.78	0.48
1:B:696:GLU:HB2	1:B:699:ILE:HG22	1.94	0.48
1:B:490:TYR:CE2	1:B:524:CYS:HB3	2.47	0.48
1:B:60:GLY:O	1:B:64:GLU:HG3	2.12	0.48
1:A:132:MET:CE	1:A:136:ILE:HG13	2.44	0.48
1:B:471:ASN:HD22	1:B:472:TYR:N	2.10	0.48
1:A:186:LEU:HD13	1:A:187:TYR:CE1	2.48	0.48
1:B:186:LEU:HD13	1:B:187:TYR:CZ	2.48	0.48
1:B:550:GLU:OE1	1:B:550:GLU:HA	2.12	0.48
1:A:165:LEU:HD22	1:A:168:LEU:HD11	1.95	0.48
1:B:222:GLU:CD	1:B:595:ARG:HH22	2.16	0.48
1:B:33:TYR:CE1	1:B:35:PRO:HG3	2.48	0.48
1:B:381:LEU:HD22	1:B:384:LYS:HD2	1.95	0.48
1:B:180:ASP:HB3	1:B:183:ARG:HG3	1.95	0.48
1:B:748:GLN:O	1:B:752:THR:HG23	2.13	0.48
1:A:158:ARG:HG2	1:A:456:MET:CE	2.44	0.48
1:B:33:TYR:HA	1:B:285:VAL:HG22	1.96	0.48
1:B:468:ASP:O	1:B:545:LYS:HG3	2.14	0.48
1:A:372:THR:CG2	1:A:400:GLU:HG3	2.44	0.48
1:A:400:GLU:OE2	1:A:704:HIS:HD2	1.97	0.48
1:A:132:MET:HE3	1:A:132:MET:O	2.13	0.47
1:A:719:MET:SD	1:A:751:ILE:HD13	2.54	0.47
1:A:381:LEU:HD22	1:A:384:LYS:HD2	1.96	0.47
1:A:548:ARG:HG3	1:A:548:ARG:NH1	2.29	0.47
1:B:445:ALA:HA	1:B:482:PHE:CD2	2.50	0.47
1:A:526:ILE:CG1	1:A:601:GLN:HE21	2.28	0.47
1:B:406:ARG:N	1:B:407:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ILE:HG13	1:A:601:GLN:NE2	2.29	0.47
1:B:158:ARG:HG2	1:B:456:MET:HE2	1.96	0.47
1:B:19:TRP:HD1	1:B:27:ASP:OD1	1.96	0.47
1:B:313:ARG:HG2	1:B:368:GLU:O	2.14	0.47
1:A:468:ASP:O	1:A:545:LYS:HG3	2.15	0.47
1:A:748:GLN:O	1:A:752:THR:HG23	2.15	0.47
1:A:112:PHE:HD2	1:A:141:ARG:CZ	2.26	0.47
1:B:526:ILE:HG13	1:B:601:GLN:NE2	2.30	0.47
1:B:636:MET:HB2	1:B:639:ARG:HD2	1.97	0.47
1:A:33:TYR:HA	1:A:285:VAL:HG22	1.97	0.47
1:A:60:GLY:O	1:A:64:GLU:HG3	2.15	0.47
1:B:468:ASP:O	1:B:546:PRO:HD2	2.15	0.47
1:A:186:LEU:HD13	1:A:187:TYR:CZ	2.50	0.46
1:B:16:LYS:O	1:B:31:LYS:HD3	2.15	0.46
1:B:372:THR:CG2	1:B:400:GLU:HG3	2.45	0.46
1:A:490:TYR:CE2	1:A:524:CYS:HB3	2.50	0.46
1:B:719:MET:SD	1:B:751:ILE:HD13	2.55	0.46
1:B:328:SER:CB	1:B:746:GLN:NE2	2.76	0.46
1:B:386:PHE:O	1:B:390:VAL:HG23	2.16	0.46
1:A:636:MET:HB2	1:A:639:ARG:HD2	1.96	0.46
1:A:17:GLY:HA3	1:A:31:LYS:HD2	1.98	0.46
1:A:406:ARG:N	1:A:407:PRO:HD2	2.31	0.46
1:B:409:PHE:CE2	1:B:422:PRO:HB2	2.49	0.46
1:B:537:SER:OG	1:B:564:PRO:HG2	2.16	0.46
1:A:159:CYS:HB3	1:A:165:LEU:HB2	1.98	0.46
1:B:159:CYS:HB3	1:B:165:LEU:HB2	1.97	0.46
1:B:360:LEU:HD23	1:B:390:VAL:CG1	2.46	0.46
1:B:134:LYS:O	1:B:138:THR:HG23	2.16	0.46
1:B:455:LYS:HG2	1:B:553:LEU:CD2	2.46	0.46
1:B:414:TYR:HA	1:B:424:ILE:HA	1.98	0.46
1:A:158:ARG:HG2	1:A:456:MET:HE1	1.99	0.45
1:B:278:ARG:HG3	4:B:2208:HOH:O	2.15	0.45
1:B:548:ARG:HG3	1:B:548:ARG:NH1	2.27	0.45
1:A:313:ARG:HG2	1:A:368:GLU:O	2.15	0.45
1:B:159:CYS:HB3	1:B:164:VAL:HG13	1.99	0.45
1:A:386:PHE:O	1:A:390:VAL:HG23	2.16	0.45
1:A:601:GLN:HG2	1:A:602:SER:N	2.32	0.45
1:B:112:PHE:HD2	1:B:141:ARG:CZ	2.28	0.45
1:B:442:MET:HE1	1:B:536:LEU:HG	1.98	0.45
1:A:445:ALA:HA	1:A:482:PHE:CD2	2.52	0.45
1:A:537:SER:OG	1:A:564:PRO:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:OE2	1:B:595:ARG:NH2	2.50	0.45
1:B:400:GLU:OE2	1:B:704:HIS:HD2	2.00	0.45
1:B:526:ILE:CG1	1:B:601:GLN:HE21	2.29	0.45
1:A:159:CYS:HB3	1:A:164:VAL:HG13	1.97	0.45
1:A:230:LEU:O	1:A:233:MET:HB2	2.16	0.45
1:A:538:ALA:O	1:A:542:ALA:HB3	2.17	0.45
1:B:160:ARG:HA	1:B:165:LEU:O	2.17	0.45
1:B:265:ALA:HB1	1:B:510:LEU:HD11	1.99	0.45
1:B:17:GLY:HA3	1:B:31:LYS:HD2	1.99	0.45
1:A:414:TYR:HA	1:A:424:ILE:HA	1.98	0.45
1:B:165:LEU:HD22	1:B:168:LEU:HD11	1.98	0.45
1:A:353:SER:O	1:A:357:LEU:HD13	2.17	0.44
1:A:409:PHE:CE2	1:A:422:PRO:HB2	2.50	0.44
1:B:79:SER:HB3	1:B:110:ILE:HD13	2.00	0.44
1:A:112:PHE:CD1	4:A:2137:HOH:O	2.49	0.44
1:A:16:LYS:O	1:A:31:LYS:HD3	2.17	0.44
1:B:601:GLN:HG2	1:B:602:SER:N	2.32	0.44
1:A:309:VAL:O	1:A:313:ARG:HG3	2.18	0.44
1:B:538:ALA:O	1:B:542:ALA:HB3	2.17	0.44
1:A:360:LEU:HD23	1:A:390:VAL:CG1	2.48	0.44
1:B:73:PHE:CZ	1:B:127:ARG:HG3	2.52	0.44
1:B:353:SER:O	1:B:357:LEU:HD13	2.17	0.44
1:A:73:PHE:CZ	1:A:127:ARG:HG3	2.51	0.44
1:A:160:ARG:HA	1:A:165:LEU:O	2.18	0.44
1:A:713:GLU:OE1	1:A:713:GLU:N	2.50	0.44
1:B:114:GLY:HA2	1:B:143:THR:CB	2.48	0.44
1:B:481:HIS:O	1:B:484:ASP:HB2	2.17	0.44
1:B:610:VAL:HA	1:B:628:PRO:HB3	1.99	0.44
1:B:677:ASP:OD1	1:B:680:VAL:HG23	2.18	0.44
1:A:241:GLY:HA3	2:A:1001:PGE:H4	1.99	0.44
1:A:468:ASP:O	1:A:546:PRO:HD2	2.17	0.44
1:B:578:VAL:O	1:B:582:GLU:HG3	2.18	0.44
1:B:526:ILE:HD11	1:B:584:PHE:CE2	2.52	0.44
1:A:526:ILE:HD11	1:A:584:PHE:CE2	2.53	0.44
1:A:712:ARG:HH11	1:A:712:ARG:HG3	1.83	0.44
1:B:310:MET:O	1:B:313:ARG:HB2	2.18	0.44
1:A:427:LYS:HG2	1:A:515:ASP:OD1	2.18	0.43
1:A:677:ASP:OD1	1:A:680:VAL:HG23	2.18	0.43
1:B:556:ASP:OD1	1:B:557:PHE:N	2.51	0.43
1:B:710:MET:HB2	1:B:714:MET:CE	2.49	0.43
1:A:265:ALA:HB1	1:A:510:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:VAL:O	1:A:582:GLU:HG3	2.18	0.43
1:B:713:GLU:OE1	1:B:713:GLU:N	2.51	0.43
1:A:114:GLY:HA2	1:A:143:THR:CB	2.48	0.43
1:A:54:TRP:HE1	1:A:727:GLN:HE22	1.67	0.43
1:B:559:ILE:HD12	1:B:559:ILE:H	1.84	0.43
1:A:455:LYS:HG2	1:A:553:LEU:CD2	2.49	0.43
1:A:710:MET:HB2	1:A:714:MET:CE	2.49	0.43
1:A:733:SER:HB2	4:A:2076:HOH:O	2.18	0.43
1:A:640:ASP:OD1	1:A:754:THR:HG21	2.19	0.43
1:A:610:VAL:HA	1:A:628:PRO:HB3	2.00	0.43
1:A:132:MET:HE3	1:A:136:ILE:HG13	2.00	0.43
1:A:481:HIS:O	1:A:484:ASP:HB2	2.18	0.43
1:B:230:LEU:O	1:B:233:MET:HB2	2.19	0.43
1:A:134:LYS:O	1:A:138:THR:HG23	2.18	0.43
1:A:650:SER:O	1:A:653:LYS:HB2	2.19	0.43
1:A:559:ILE:HD12	1:A:559:ILE:H	1.83	0.42
1:A:732:VAL:HG23	1:A:735:TYR:CE2	2.54	0.42
1:B:309:VAL:O	1:B:313:ARG:HG3	2.18	0.42
1:A:526:ILE:CG1	1:A:601:GLN:NE2	2.82	0.42
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.90	0.42
1:B:146:GLN:HG2	4:B:2158:HOH:O	2.19	0.42
1:B:158:ARG:NH1	4:B:2179:HOH:O	2.51	0.42
1:B:86:ALA:HA	1:B:240:TYR:CZ	2.55	0.42
1:B:531:VAL:HG12	1:B:636:MET:CG	2.50	0.42
1:B:64:GLU:O	1:B:68:HIS:N	2.53	0.42
1:B:640:ASP:OD1	1:B:754:THR:HG21	2.19	0.42
1:B:333:TRP:HB3	1:B:418:CYS:HA	2.00	0.42
1:A:110:ILE:C	4:A:2137:HOH:O	2.58	0.42
1:A:385:LYS:HE3	1:A:683:THR:HG23	2.02	0.42
1:A:333:TRP:HB3	1:A:418:CYS:HA	2.01	0.42
1:B:650:SER:O	1:B:653:LYS:HB2	2.19	0.42
1:B:712:ARG:HH11	1:B:712:ARG:HG3	1.85	0.42
1:A:748:GLN:NE2	1:A:751:ILE:HD11	2.34	0.42
1:B:732:VAL:HG23	1:B:735:TYR:CE2	2.55	0.42
1:B:342:GLY:HA3	4:B:2172:HOH:O	2.19	0.41
1:B:421:SER:HA	1:B:422:PRO:HD2	1.93	0.41
1:B:720:GLU:C	1:B:721:ASN:HD22	2.24	0.41
1:A:79:SER:HB3	1:A:110:ILE:HD13	2.02	0.41
1:A:720:GLU:C	1:A:721:ASN:HD22	2.23	0.41
1:A:435:ARG:HB3	1:A:435:ARG:HE	1.72	0.41
1:B:748:GLN:NE2	1:B:751:ILE:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:MET:HG2	1:B:171:ALA:O	2.21	0.41
1:A:86:ALA:HA	1:A:240:TYR:CZ	2.55	0.41
1:B:548:ARG:HD3	1:B:552:GLY:O	2.21	0.41
1:A:281:THR:HB	4:A:2005:HOH:O	2.20	0.41
1:A:442:MET:HE1	1:A:536:LEU:HG	2.03	0.41
1:A:548:ARG:HD3	1:A:552:GLY:O	2.20	0.41
1:B:165:LEU:HA	1:B:165:LEU:HD23	1.79	0.41
1:A:38:GLY:C	1:A:382:ASN:HD22	2.24	0.41
1:B:196:LYS:HA	1:B:196:LYS:HD3	1.88	0.41
1:A:211:VAL:O	1:A:216:THR:HG21	2.20	0.41
1:B:427:LYS:HG2	1:B:515:ASP:OD1	2.21	0.41
1:A:556:ASP:OD1	1:A:557:PHE:N	2.50	0.40
1:B:526:ILE:CG1	1:B:601:GLN:NE2	2.84	0.40
1:A:47:THR:HG23	4:A:2054:HOH:O	2.21	0.40
1:A:388:ALA:O	1:A:392:ILE:HG13	2.22	0.40
1:A:531:VAL:HG12	1:A:636:MET:CG	2.51	0.40
1:B:211:VAL:O	1:B:216:THR:HG21	2.20	0.40
1:B:398:GLN:HB3	1:B:731:ARG:NH2	2.37	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)
2:A:1001:PGE:C1	2:A:1001:PGE:O1[8_776]	1.46	0.74

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	754/759 (99%)	708 (94%)	44 (6%)	2 (0%)	41	66
1	B	754/759 (99%)	706 (94%)	46 (6%)	2 (0%)	41	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1508/1518 (99%)	1414 (94%)	90 (6%)	4 (0%)	41 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	ILE
1	A	733	SER
1	B	606	ILE
1	B	733	SER

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	635/638 (100%)	606 (95%)	29 (5%)	27 54
1	B	635/638 (100%)	607 (96%)	28 (4%)	28 56
All	All	1270/1276 (100%)	1213 (96%)	57 (4%)	27 55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	40	GLU
1	A	75	THR
1	A	117	MET
1	A	126	ASN
1	A	152	TYR
1	A	165	LEU
1	A	186	LEU
1	A	207	LEU
1	A	216	THR
1	A	252	GLN
1	A	257	TRP
1	A	260	PHE
1	A	326	LEU

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	360	LEU
1	A	381	LEU
1	A	393	ASP
1	A	435	ARG
1	A	438	LEU
1	A	471	ASN
1	A	479	MET
1	A	490	TYR
1	A	550	GLU
1	A	573	VAL
1	A	595	ARG
1	A	660	LYS
1	A	710	MET
1	A	735	TYR
1	B	5	GLU
1	B	40	GLU
1	B	75	THR
1	B	117	MET
1	B	126	ASN
1	B	152	TYR
1	B	186	LEU
1	B	207	LEU
1	B	216	THR
1	B	252	GLN
1	B	257	TRP
1	B	260	PHE
1	B	326	LEU
1	B	348	LEU
1	B	360	LEU
1	B	381	LEU
1	B	393	ASP
1	B	435	ARG
1	B	438	LEU
1	B	471	ASN
1	B	479	MET
1	B	490	TYR
1	B	550	GLU
1	B	573	VAL
1	B	595	ARG
1	B	660	LYS
1	B	710	MET

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Mol	Chain	Res	Type
1	B	735	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	126	ASN
1	A	358	ASN
1	A	382	ASN
1	A	410	ASN
1	A	430	GLN
1	A	471	ASN
1	A	489	GLN
1	A	589	GLN
1	A	601	GLN
1	A	684	ASN
1	A	711	ASN
1	A	721	ASN
1	A	727	GLN
1	A	748	GLN
1	B	4	ASN
1	B	126	ASN
1	B	358	ASN
1	B	382	ASN
1	B	410	ASN
1	B	430	GLN
1	B	471	ASN
1	B	589	GLN
1	B	601	GLN
1	B	684	ASN
1	B	711	ASN
1	B	721	ASN
1	B	727	GLN
1	B	748	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)

3 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	PGE	A	1001	-	9,9,9	0.82	0	8,8,8	0.76	0
3	PYR	A	2001	-	2,5,5	1.16	0	2,6,6	0.53	0
3	PYR	B	2002	-	2,5,5	1.18	0	2,6,6	0.61	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	PGE	A	1001	-	-	2/7/7/7	-
3	PYR	A	2001	-	-	0/0/4/4	-
3	PYR	B	2002	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PGE	O2-C3-C4-O3
2	A	1001	PGE	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PGE	1	1
3	A	2001	PYR	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	756/759 (99%)	-0.36	9 (1%)	79	80	25, 43, 74, 96	0
1	B	756/759 (99%)	-0.32	13 (1%)	70	72	25, 45, 74, 95	0
All	All	1512/1518 (99%)	-0.34	22 (1%)	73	76	25, 44, 74, 96	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	468	ASP	4.1
1	B	550	GLU	3.5
1	B	699	ILE	3.3
1	A	550	GLU	3.1
1	B	641	GLN	3.0
1	A	6	LYS	3.0
1	A	721	ASN	2.7
1	B	553	LEU	2.7
1	B	5	GLU	2.7
1	A	4	ASN	2.6
1	A	699	ILE	2.6
1	B	676	LYS	2.5
1	A	720	GLU	2.4
1	B	698	SER	2.4
1	B	560	GLU	2.4
1	B	467	GLY	2.2
1	B	461	LYS	2.1
1	A	698	SER	2.1
1	A	696	GLU	2.1
1	B	541	TYR	2.1
1	A	744	LYS	2.1
1	B	543	LYS	2.1

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PGE	A	1001	10/10	0.90	0.22	46,55,61,63	1
3	PYR	B	2002	6/6	0.94	0.17	46,47,50,50	0
3	PYR	A	2001	6/6	0.97	0.12	32,33,33,35	0

6.5 Other polymers (i)

There are no such residues in this entry.