

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8H1R
Title	:	Crystal structure of LptDE-YifL complex
Authors	:	Luo, Q.; Huang, Y.
Deposited on	:	2022-10-03
Resolution	:	2.98 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.98 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of cha	ain
1	А	924	5%	· 20%
1	D	924	59%	25% · 15%
2	В	207	4% 66%	16% · 17%
2	Е	207	<u>4%</u> 62%	21% 17%
3	С	67	4% 13% • 82%	
3	F	67	6% 13% • 82%	



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
4	PCJ	А	1001	-	-	Х	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15559 atoms, of which 210 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	736	Total 5976	C 3778	N 1035	0 1148	S 15	0	0	0
1	D	789	Total 6387	C 4041	N 1106	0 1223	S 17	0	0	0

• Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	В	179	Total	С	Ν	Ο	S	0	0	0
	D	172	1341	818	247	272	4	0	0	0
0	F	179	Total	С	Ν	0	S	0	0	0
	Ľ	172	1341	818	247	272	4	0		U

• Molecule 3 is a protein called Uncharacterized lipoprotein YifL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	12	Total 90	С 62	N 13	O 15	0	0	0
3	F	12	Total 90	C 62	N 13	O 15	0	0	0

• Molecule 4 is (2R)-3-{[(2S)-3-HYDROXY-2-(PALMITOYLAMINO)PROPYL]THIO}PRO PANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PCJ) (formula: C₅₄H₁₀₅NO₆S) (labeled as "Ligand of Interest" by depositor).





PCJ	

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
4	Λ	1	Total	С	Η	Ν	0	\mathbf{S}	0	0	
4	Л	1	167	54	105	1	6	1	0	0	
4	Л	1	Total	С	Η	Ν	0	\mathbf{S}	0	0	
4	D	T	167	54	105	1	6	1	0	0	



3 Residue-property plots (i)

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



• Molecule 1: LPS-assembly protein LptD

• Molecule 1: LPS-assembly protein LptD











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	93.85Å 140.47Å 133.18Å	Depositor
a, b, c, α , β , γ	90.00° 104.39° 90.00°	Depositor
Bosolution (Å)	43.25 - 2.98	Depositor
Resolution (A)	43.25 - 2.98	EDS
% Data completeness	97.2 (43.25-2.98)	Depositor
(in resolution range)	97.2 (43.25-2.98)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.20 (at 2.95 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.234 , 0.264	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.235 , 0.262	DCC
R_{free} test set	3322 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	72.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 50.0	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15559	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 23.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3420e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: PCJ

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).

Mal	Chain	Bond	lengths	Bo	ond angles
INIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.51	0/6127	0.75	1/8307~(0.0%)
1	D	0.48	0/6549	0.70	0/8878
2	В	0.50	0/1353	0.73	1/1826~(0.1%)
2	Е	0.50	0/1353	0.68	0/1826
3	С	0.68	0/94	0.79	0/128
3	F	0.51	0/94	0.68	0/128
All	All	0.50	0/15570	0.72	2/21093~(0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	6	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	А	279	LEU	CB-CG-CD2	-5.17	102.20	111.00

There are no chirality outliers.

There are no planarity outliers.

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	А	5976	0	5674	177	0
1	D	6387	0	6078	174	0
2	В	1341	0	1319	27	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Е	1341	0	1319	32	0
3	С	90	0	88	5	0
3	F	90	0	88	3	0
4	А	62	105	105	26	0
4	D	62	105	105	4	0
All	All	15349	210	14776	405	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:629:THR:HG22	1:D:687:ARG:H	1.34	0.93
1:D:487:PRO:HD2	1:D:512:ARG:HB3	1.50	0.92
4:A:1001:PCJ:HN	3:C:21:GLY:N	1.69	0.89
1:A:613:LEU:O	1:A:632:PRO:HD2	1.77	0.85
1:A:487:PRO:HD2	1:A:512:ARG:HB3	1.59	0.85
1:D:376:THR:HG22	1:D:377:HIS:H	1.41	0.84
1:A:350:PRO:HG2	3:C:29:PRO:HG3	1.58	0.84
1:D:533:ARG:HD3	1:D:534:PRO:HD2	1.61	0.83
1:D:162:LYS:HG2	1:D:177:GLY:HA3	1.62	0.81
1:A:313:ILE:HD11	4:A:1001:PCJ:CB	2.12	0.79
1:D:326:LEU:HB2	1:D:343:PRO:HG2	1.63	0.79
1:A:376:THR:HG22	1:A:377:HIS:H	1.48	0.79
1:A:864:LEU:HD13	1:A:890:LEU:HD13	1.65	0.78
1:D:553:PRO:HD2	1:D:572:TYR:O	1.82	0.78
1:A:773:ALA:O	1:A:774:ILE:HD13	1.84	0.77
1:A:260:ILE:HD11	1:A:286:LEU:HD12	1.68	0.76
2:B:68:THR:HG22	2:B:69:GLY:H	1.51	0.75
1:A:836:ARG:NH1	1:A:848:GLU:OE1	2.21	0.73
1:A:313:ILE:HD11	4:A:1001:PCJ:HB2	1.70	0.73
1:D:649:VAL:HG13	1:D:652:THR:HB	1.70	0.73
1:A:398:PHE:CE1	1:A:876:ALA:HB2	2.24	0.72
1:A:357:TYR:HB2	1:A:369:GLU:HB2	1.70	0.72
1:A:328:PRO:HG3	4:A:1001:PCJ:O3	1.89	0.71
1:A:870:LEU:HD13	1:A:882:GLU:HG3	1.72	0.71
1:A:867:ARG:HD2	1:A:908:PHE:CE2	2.25	0.71
2:B:82:ILE:HG13	2:B:130:LEU:HD13	1.71	0.71
1:A:819:HIS:CD2	1:A:839:TYR:HB3	2.25	0.71
1:A:326:LEU:HB2	1:A:343:PRO:HG2	1.73	0.70



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:203:GLU:HG2	1:D:223:GLN:HG2	1.73	0.70
1:A:793:TYR:HA	1:A:816:ILE:O	1.91	0.70
1:A:845:ARG:NH1	1:A:882:GLU:OE2	2.24	0.70
1:A:314:TYR:CE1	4:A:1001:PCJ:H642	2.27	0.69
1:A:649:VAL:HG13	1:A:652:THR:HB	1.72	0.69
1:D:615:PHE:HB2	1:D:630:LEU:HB3	1.75	0.69
1:A:305:PHE:HD2	4:A:1001:PCJ:H312	1.55	0.69
1:D:863:ARG:NH2	1:D:906:GLU:OE2	2.24	0.68
1:D:376:THR:HG22	1:D:377:HIS:N	2.09	0.68
1:A:353:ASP:OD2	1:A:373:ARG:NH1	2.26	0.68
2:E:9:LEU:HD12	2:E:9:LEU:H	1.58	0.67
1:A:828:VAL:HG13	1:A:829:PRO:HD2	1.77	0.67
1:D:371:GLU:OE2	1:D:373:ARG:HD2	1.95	0.67
2:E:2:CYS:SG	2:E:3:GLY:N	2.67	0.67
1:D:793:TYR:HA	1:D:816:ILE:O	1.94	0.67
1:A:328:PRO:HD3	4:A:1001:PCJ:H452	1.77	0.66
1:A:249:ALA:HB2	1:A:262:LEU:HB3	1.77	0.66
1:D:212:ASP:OD2	1:D:254:ARG:NH1	2.27	0.66
1:D:819:HIS:CD2	1:D:839:TYR:HB3	2.30	0.66
1:D:647:LEU:O	1:D:673:ARG:NH2	2.29	0.66
1:A:615:PHE:CE1	2:B:6:LEU:CD2	2.79	0.65
2:E:123:ARG:HA	2:E:126:MET:HE3	1.77	0.65
1:A:250:LEU:O	1:A:250:LEU:HD23	1.97	0.64
4:A:1001:PCJ:C1	4:A:1001:PCJ:H1	2.25	0.64
1:D:490:THR:HG22	1:D:509:GLU:HG3	1.79	0.64
1:D:822:SER:HB3	1:D:836:ARG:HG3	1.78	0.64
1:D:868:TYR:CE1	1:D:884:ALA:HB1	2.33	0.64
1:A:195:LEU:O	1:A:196:HIS:ND1	2.30	0.64
1:D:215:MET:HG2	1:D:254:ARG:HH21	1.64	0.62
1:A:556:SER:HB3	1:A:569:THR:HG23	1.82	0.62
1:A:681:SER:OG	1:A:704:ILE:HG12	1.99	0.62
1:D:300:LEU:O	1:D:307:VAL:HG12	2.00	0.62
1:A:208:VAL:HG21	1:A:222:ALA:HB2	1.82	0.61
1:A:376:THR:HG22	1:A:377:HIS:N	2.15	0.61
1:A:660:ASP:OD2	2:B:103:LYS:HE3	2.00	0.61
1:D:144:PRO:HB2	1:D:182:ARG:HH22	1.64	0.61
1:D:850:PHE:CE2	1:D:913:ILE:HD13	2.36	0.61
1:D:819:HIS:CE1	1:D:821:PHE:CE2	2.89	0.61
1:D:617:ARG:NH2	1:D:628:GLN:OE1	2.31	0.61
1:A:305:PHE:HD2	4:A:1001:PCJ:C31	2.14	0.60
1:D:789:VAL:HG13	1:D:821:PHE:CD1	2.36	0.60



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:819:HIS:ND1	1:D:821:PHE:CE2	2.69	0.60
1:A:328:PRO:CD	4:A:1001:PCJ:H452	2.31	0.60
1:D:332:SER:HA	1:D:337:GLY:O	2.01	0.60
1:A:615:PHE:CE1	2:B:6:LEU:HD23	2.37	0.60
1:A:610:ASP:CG	1:A:633:ARG:HH21	2.05	0.60
1:D:341:VAL:HG22	1:D:359:ARG:HG2	1.84	0.60
1:A:314:TYR:CD1	4:A:1001:PCJ:H642	2.37	0.60
1:D:353:ASP:OD1	1:D:373:ARG:HD3	2.00	0.60
1:D:461:ASP:O	2:E:32:ARG:HD2	2.01	0.60
1:A:359:ARG:NE	1:A:369:GLU:OE2	2.28	0.59
1:A:502:MET:HG2	1:A:503:GLN:N	2.17	0.59
1:A:642:LYS:O	1:A:644:GLN:HG3	2.01	0.59
1:D:301:ARG:HA	1:D:305:PHE:O	2.02	0.59
1:A:321:ARG:NH1	1:A:345:TYR:OH	2.35	0.59
2:B:68:THR:HG22	2:B:69:GLY:N	2.17	0.59
1:D:629:THR:HG22	1:D:687:ARG:N	2.14	0.59
1:A:606:LEU:HD11	1:A:665:GLU:HB2	1.85	0.58
1:D:877:PHE:O	1:D:879:VAL:HG23	2.03	0.58
1:D:130:ILE:H	1:D:130:ILE:HD12	1.68	0.58
1:A:249:ALA:CB	1:A:262:LEU:HB3	2.34	0.58
1:A:828:VAL:CG1	1:A:829:PRO:HD2	2.34	0.57
1:D:769:GLU:HG3	1:D:796:ASP:HB3	1.86	0.57
1:D:669:THR:HG21	2:E:118:GLU:HA	1.86	0.57
1:D:789:VAL:HG13	1:D:821:PHE:CE1	2.39	0.57
4:D:1001:PCJ:C	3:F:21:GLY:HA2	2.34	0.57
1:A:321:ARG:HH21	1:A:350:PRO:HA	1.69	0.57
1:A:557:LEU:O	1:A:568:PRO:HD2	2.05	0.57
1:D:328:PRO:HD3	4:D:1001:PCJ:C45	2.35	0.57
1:D:828:VAL:HG13	1:D:829:PRO:HD2	1.85	0.57
1:D:165:ARG:HG2	1:D:166:TYR:H	1.69	0.57
1:D:909:LEU:HA	1:D:913:ILE:HD12	1.86	0.56
2:B:53:LEU:HD22	2:B:138:LEU:HD11	1.86	0.56
1:D:294:THR:HG22	1:D:314:TYR:HB3	1.86	0.56
2:E:68:THR:HG22	2:E:69:GLY:H	1.70	0.56
2:E:79:THR:HG23	2:E:102:GLN:HG2	1.86	0.56
1:A:179:VAL:HG11	1:A:193:ALA:HB2	1.87	0.56
1:D:868:TYR:HE1	1:D:884:ALA:HB1	1.68	0.56
1:D:850:PHE:CZ	1:D:913:ILE:HD13	2.41	0.56
1:D:410:LEU:HD23	1:D:424:VAL:HG11	1.88	0.55
1:D:446:SER:OG	1:D:447:THR:N	2.27	0.55
1:A:579:LEU:HD11	1:A:648:PRO:HD3	1.89	0.55



	page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:648:PRO:HG2	1:A:650:PHE:CE2	2.42	0.55
1:D:459:ARG:NH1	2:E:25:ASN:OD1	2.30	0.55
1:D:579:LEU:HD11	1:D:648:PRO:HD3	1.88	0.55
1:A:819:HIS:CE1	1:A:821:PHE:CE2	2.94	0.55
1:A:407:LEU:C	1:A:407:LEU:HD23	2.27	0.55
1:A:610:ASP:OD2	1:A:633:ARG:NH2	2.40	0.54
1:D:210:LEU:HD23	1:D:211:ARG:N	2.22	0.54
1:A:609:VAL:O	1:A:635:MET:HA	2.07	0.54
1:D:350:PRO:HB3	3:F:27:TYR:CZ	2.42	0.54
1:D:486:LEU:HB2	1:D:487:PRO:HD3	1.88	0.54
1:D:133:TYR:CD2	1:D:830:GLN:HG2	2.43	0.54
1:D:864:LEU:HD11	1:D:888:ILE:HD11	1.90	0.54
1:A:706:TYR:CG	1:A:710:ARG:NH1	2.76	0.54
2:B:2:CYS:SG	2:B:3:GLY:N	2.80	0.54
1:D:135:GLY:N	1:D:271:GLU:OE2	2.35	0.54
1:D:212:ASP:OD1	1:D:213:LYS:N	2.37	0.54
1:A:398:PHE:CD1	1:A:876:ALA:HB2	2.42	0.54
1:D:328:PRO:HD3	4:D:1001:PCJ:H451	1.90	0.54
1:D:864:LEU:HD12	1:D:889:PHE:O	2.06	0.54
1:A:794:ARG:HD2	2:B:75:GLU:OE2	2.07	0.54
2:E:105:TYR:CZ	2:E:119:ALA:HB2	2.43	0.54
1:D:353:ASP:OD2	1:D:373:ARG:NH1	2.42	0.53
1:D:794:ARG:HD2	2:E:75:GLU:OE2	2.08	0.53
1:A:819:HIS:NE2	1:A:839:TYR:HB3	2.22	0.53
1:D:652:THR:HA	1:D:669:THR:O	2.09	0.53
1:D:829:PRO:O	1:D:830:GLN:HB2	2.08	0.53
1:A:777:TYR:CE1	1:A:779:PRO:HG3	2.44	0.53
4:A:1001:PCJ:N	3:C:21:GLY:N	2.49	0.53
1:D:718:THR:HG23	1:D:721:ASP:H	1.74	0.53
1:A:321:ARG:NH2	1:A:350:PRO:HA	2.23	0.53
1:A:822:SER:HB3	1:A:836:ARG:HG3	1.89	0.53
1:D:144:PRO:HD2	1:D:182:ARG:HH12	1.72	0.53
1:A:617:ARG:NH2	1:A:628:GLN:OE1	2.39	0.53
1:A:270:CYS:HB3	1:A:274:SER:HB3	1.91	0.53
1:A:909:LEU:HD23	1:A:916:TYR:CE2	2.44	0.52
1:D:133:TYR:CE2	1:D:830:GLN:HG2	2.44	0.52
1:A:212:ASP:OD1	1:A:213:LYS:N	2.34	0.52
1:A:657:PHE:HE2	1:A:742:ALA:HB2	1.74	0.52
1:A:533:ARG:HD3	1:A:534:PRO:HD2	1.90	0.52
1:D:357:TYR:HB2	1:D:369:GLU:HB2	1.92	0.52
1:A:698:SER:O	1:A:745:GLY:HA2	2.10	0.52



	page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:374:TYR:CZ	1:D:381:GLY:HA3	2.44	0.52
1:D:524:ASN:N	1:D:528:SER:O	2.37	0.52
1:D:819:HIS:NE2	1:D:839:TYR:HB3	2.25	0.52
1:A:305:PHE:CD2	4:A:1001:PCJ:H312	2.42	0.51
1:A:682:LEU:HD12	1:A:705:TYR:CE2	2.45	0.51
1:A:704:ILE:HB	1:A:739:SER:HB3	1.91	0.51
1:D:777:TYR:CE1	1:D:779:PRO:HD3	2.45	0.51
1:D:341:VAL:HG21	1:D:359:ARG:NH1	2.25	0.51
1:A:502:MET:HE3	1:A:555:MET:HB3	1.91	0.51
1:D:199:GLU:OE2	1:D:225:GLN:NE2	2.43	0.51
1:A:250:LEU:HD23	1:A:250:LEU:C	2.31	0.51
2:B:101:VAL:HG12	2:B:130:LEU:HD21	1.91	0.51
1:A:385:ALA:HA	1:A:407:LEU:O	2.10	0.51
1:A:605:PRO:HD2	1:A:640:PRO:CG	2.40	0.51
1:A:669:THR:HG21	2:B:118:GLU:HA	1.93	0.51
1:A:682:LEU:HD12	1:A:705:TYR:HE2	1.76	0.51
3:C:22:LEU:C	3:C:22:LEU:HD23	2.31	0.51
1:D:487:PRO:CD	1:D:512:ARG:HB3	2.30	0.51
4:A:1001:PCJ:H1	4:A:1001:PCJ:H2	1.92	0.51
2:E:101:VAL:HG12	2:E:130:LEU:HD21	1.92	0.51
1:A:269:ARG:HD3	1:A:896:GLY:HA3	1.93	0.50
2:E:66:SER:HB2	2:E:75:GLU:HB2	1.92	0.50
1:D:339:THR:HA	1:D:360:TYR:O	2.11	0.50
1:D:614:TYR:HD1	1:D:631:GLU:HG2	1.76	0.50
1:A:773:ALA:C	1:A:774:ILE:HD13	2.32	0.50
1:A:819:HIS:ND1	1:A:821:PHE:CE2	2.80	0.50
1:D:248:SER:H	1:D:266:THR:HB	1.76	0.50
2:B:21:VAL:HG23	2:B:45:VAL:HG13	1.93	0.50
1:A:788:ASN:HB2	1:A:822:SER:OG	2.12	0.50
1:A:910:ASP:OD2	1:A:917:ARG:NH1	2.36	0.49
1:D:838:GLN:NE2	2:E:67:TYR:HE2	2.10	0.49
1:D:576:LYS:NZ	1:D:599:ASN:HB3	2.28	0.49
1:D:476:THR:OG1	1:D:477:THR:N	2.44	0.49
1:D:160:SER:HB3	1:D:180:VAL:CG2	2.42	0.49
2:E:87:VAL:HG22	2:E:93:VAL:HG12	1.94	0.49
1:D:118:PRO:O	1:D:123:THR:OG1	2.21	0.49
1:A:348:LEU:O	1:A:349:ALA:HB2	2.13	0.49
1:A:462:THR:HG22	1:A:494:PHE:CZ	2.47	0.49
1:D:321:ARG:HH12	1:D:350:PRO:HA	1.78	0.49
2:B:32:ARG:NH1	2:B:36:GLU:OE2	2.46	0.49
1:D:144:PRO:HD2	1:D:182:ARG:NH1	2.28	0.48



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:617:ARG:HG2	1:D:619:THR:HG23	1.95	0.48
1:A:570:LEU:HD11	1:D:502:MET:HE1	1.94	0.48
1:A:625:PRO:HD2	1:A:691:GLU:OE2	2.12	0.48
1:A:486:LEU:CB	1:A:487:PRO:HD3	2.43	0.48
1:A:615:PHE:HB2	1:A:630:LEU:HB3	1.94	0.48
1:A:633:ARG:HG3	1:A:663:TRP:CH2	2.49	0.48
1:A:769:GLU:HG3	1:A:796:ASP:HB3	1.94	0.48
4:A:1001:PCJ:C65	4:A:1001:PCJ:HB1	2.42	0.48
1:D:208:VAL:HG12	1:D:219:GLY:O	2.13	0.48
1:D:486:LEU:CB	1:D:487:PRO:HD3	2.43	0.48
1:A:909:LEU:HD23	1:A:916:TYR:HE2	1.79	0.48
1:A:657:PHE:CE2	1:A:742:ALA:HB2	2.49	0.48
2:B:93:VAL:HG23	2:B:93:VAL:O	2.13	0.48
1:D:862:LEU:HD13	1:D:892:ILE:HG13	1.95	0.48
1:A:314:TYR:CE1	4:A:1001:PCJ:C64	2.96	0.48
2:B:82:ILE:HG13	2:B:130:LEU:CD1	2.43	0.48
1:D:161:ALA:HB1	1:D:176:ALA:O	2.14	0.48
1:A:238:TYR:CE2	1:A:262:LEU:HD13	2.49	0.48
1:D:587:THR:O	1:D:591:LYS:HB2	2.14	0.48
1:D:682:LEU:HD12	1:D:705:TYR:CE2	2.48	0.48
2:B:56:VAL:HG22	2:B:83:ASN:O	2.14	0.47
1:D:230:GLU:HA	1:D:254:ARG:O	2.14	0.47
1:A:502:MET:CG	1:A:503:GLN:N	2.77	0.47
2:E:39:GLU:C	2:E:41:SER:H	2.18	0.47
1:A:762:ASN:HB2	1:A:769:GLU:OE1	2.13	0.47
4:A:1001:PCJ:H332	4:A:1001:PCJ:H361	1.51	0.47
1:D:605:PRO:HD2	1:D:640:PRO:CG	2.45	0.47
1:D:682:LEU:HD12	1:D:705:TYR:HE2	1.79	0.47
1:A:270:CYS:SG	1:A:276:ALA:HB3	2.54	0.47
2:B:122:LEU:HD12	2:B:122:LEU:HA	1.55	0.47
2:E:68:THR:HG22	2:E:69:GLY:N	2.29	0.47
1:A:248:SER:H	1:A:266:THR:HB	1.79	0.47
1:A:850:PHE:CD1	1:A:850:PHE:C	2.88	0.47
1:A:180:VAL:C	1:A:181:LEU:HD12	2.35	0.47
1:D:247:GLY:HA3	1:D:266:THR:O	2.14	0.47
1:D:698:SER:O	1:D:745:GLY:HA2	2.15	0.47
2:E:53:LEU:HD22	2:E:138:LEU:HD11	1.96	0.47
1:A:647:LEU:O	1:A:673:ARG:NH2	2.47	0.46
1:D:282:ASN:HB2	1:D:297:ASN:HB2	1.97	0.46
1:D:741:TYR:O	1:D:760:ASN:HA	2.15	0.46
2:E:51:TYR:OH	2:E:147:ASP:OD1	2.32	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:137:ARG:O	2:B:141:LEU:HD13	2.14	0.46
1:D:348:LEU:O	1:D:349:ALA:HB2	2.15	0.46
4:D:1001:PCJ:O	3:F:21:GLY:HA2	2.14	0.46
1:A:502:MET:HE1	1:A:555:MET:SD	2.55	0.46
1:D:163:ALA:HB3	1:D:176:ALA:HB3	1.98	0.46
1:A:261:MET:O	1:A:262:LEU:HD23	2.15	0.46
1:A:260:ILE:CD1	1:A:262:LEU:HD21	2.45	0.46
1:D:773:ALA:O	1:D:774:ILE:HD13	2.16	0.46
1:D:249:ALA:CB	1:D:262:LEU:HB3	2.45	0.46
1:D:514:ASP:OD1	1:D:515:ARG:N	2.48	0.46
1:D:909:LEU:HD23	1:D:916:TYR:CE2	2.51	0.46
1:A:314:TYR:O	4:A:1001:PCJ:H651	2.15	0.46
1:A:570:LEU:HD21	1:D:502:MET:HE1	1.97	0.46
1:A:706:TYR:CD2	1:A:710:ARG:NH1	2.84	0.46
1:D:215:MET:CE	1:D:288:PRO:HG3	2.45	0.46
1:D:345:TYR:CE2	1:D:347:ASN:HB2	2.51	0.46
1:A:260:ILE:HD12	1:A:262:LEU:HD21	1.97	0.46
1:A:406:TRP:CE2	1:A:430:SER:HB3	2.51	0.46
1:D:557:LEU:O	1:D:568:PRO:HD2	2.15	0.46
1:A:328:PRO:HG3	4:A:1001:PCJ:C26	2.45	0.45
1:A:407:LEU:HD23	1:A:408:TYR:N	2.30	0.45
1:A:777:TYR:CZ	1:A:779:PRO:HG3	2.50	0.45
1:A:819:HIS:NE2	1:A:839:TYR:CB	2.79	0.45
1:A:833:VAL:HG22	1:A:834:LEU:N	2.31	0.45
1:D:146:MET:HE3	1:D:146:MET:HB3	1.85	0.45
1:D:249:ALA:HB2	1:D:262:LEU:HB3	1.97	0.45
1:D:753:TRP:HB3	1:D:777:TYR:HD1	1.81	0.45
2:E:93:VAL:HG23	2:E:93:VAL:O	2.16	0.45
1:A:502:MET:CE	1:A:555:MET:SD	3.05	0.45
1:A:634:ALA:HA	1:A:681:SER:O	2.16	0.45
1:D:277:TRP:HA	1:D:301:ARG:O	2.16	0.45
1:A:305:PHE:CD2	4:A:1001:PCJ:C31	2.98	0.45
1:D:224:VAL:HG12	1:D:225:GLN:H	1.81	0.45
1:D:823:VAL:HG22	1:D:824:ILE:N	2.30	0.45
2:B:33:GLU:HB2	2:B:131:ILE:HD11	1.97	0.45
1:A:209:LYS:HG2	1:A:218:VAL:HG12	1.99	0.45
1:A:405:ARG:HD3	1:A:431:ASP:OD1	2.17	0.45
1:A:487:PRO:HD2	1:A:512:ARG:CB	2.38	0.45
2:B:101:VAL:HG22	2:B:102:GLN:N	2.32	0.45
1:D:160:SER:HB3	1:D:180:VAL:HG22	1.99	0.45
1:A:205:VAL:HG12	1:A:206:GLY:N	2.32	0.45



	i a pageini	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:190:GLY:HA2	1:A:207:ASN:O	2.16	0.44
1:A:581:LEU:HD23	1:A:586:LYS:HG2	1.99	0.44
1:D:215:MET:HG2	1:D:260:ILE:HD11	2.00	0.44
2:B:148:GLU:HG2	2:B:151:ARG:HH21	1.82	0.44
1:D:681:SER:OG	1:D:704:ILE:HG12	2.18	0.44
1:D:814:ASP:OD1	2:E:68:THR:HG22	2.16	0.44
1:A:321:ARG:NH1	1:A:345:TYR:HH	2.15	0.44
1:A:345:TYR:CE2	1:A:347:ASN:HB2	2.52	0.44
4:A:1001:PCJ:H1	4:A:1001:PCJ:C2	2.47	0.44
4:A:1001:PCJ:HB1	4:A:1001:PCJ:H652	1.98	0.44
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.82	0.44
1:A:822:SER:HB2	1:A:913:ILE:HG12	2.00	0.44
1:D:293:GLY:O	1:D:314:TYR:HA	2.17	0.44
1:D:847:LEU:HA	1:D:870:LEU:HD22	1.99	0.44
1:D:140:GLU:HG2	1:D:241:HIS:CE1	2.53	0.43
1:D:610:ASP:OD2	1:D:633:ARG:NH2	2.49	0.43
4:A:1001:PCJ:SG	4:A:1001:PCJ:O47	2.76	0.43
1:D:327:PRO:CD	1:D:899:GLY:HA2	2.48	0.43
2:E:16:LEU:HD12	2:E:143:PRO:HG3	2.01	0.43
1:A:785:LYS:HD3	1:A:825:TRP:CZ2	2.53	0.43
1:A:850:PHE:HB2	1:A:866:ASN:O	2.18	0.43
1:D:648:PRO:HG2	1:D:650:PHE:CE2	2.54	0.43
1:A:204:LEU:HB3	1:A:222:ALA:HB3	2.01	0.43
1:D:346:PHE:HB3	1:D:348:LEU:HD21	2.01	0.43
1:D:606:LEU:HD11	1:D:665:GLU:HB2	1.99	0.43
1:D:614:TYR:CD1	1:D:631:GLU:HG2	2.52	0.43
1:A:242:LYS:HA	1:A:242:LYS:HD3	1.80	0.43
1:A:480:VAL:HG22	2:B:110:ASN:HB3	2.01	0.43
1:D:634:ALA:HA	1:D:681:SER:O	2.18	0.43
1:A:201:ARG:H	1:A:201:ARG:HD3	1.83	0.43
1:D:800:PHE:HB3	2:E:110:ASN:HB2	1.99	0.43
1:A:689:ILE:HG22	1:A:690:GLU:O	2.19	0.43
1:A:210:LEU:O	1:A:216:LEU:HD12	2.19	0.43
1:D:608:LYS:HA	1:D:636:TYR:O	2.19	0.43
1:D:847:LEU:HD23	1:D:870:LEU:HD22	2.01	0.43
2:E:103:LYS:HD3	2:E:122:LEU:HD11	2.01	0.43
2:E:133:GLN:O	2:E:137:ARG:HG3	2.19	0.43
1:A:604:LEU:O	1:A:604:LEU:HD12	2.19	0.43
1:A:794:ARG:NH1	2:B:75:GLU:OE2	2.49	0.43
1:D:508:THR:HG22	1:D:551:LEU:HD22	2.00	0.43
1:D:563:TRP:HB2	2:E:6:LEU:HD22	1.99	0.43



	A de la construction de la const	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:234:ASP:O	1:A:235:ASN:C	2.57	0.43
1:A:321:ARG:HA	3:C:22:LEU:O	2.18	0.43
2:B:31:VAL:O	2:B:35:LYS:HG3	2.18	0.43
1:D:617:ARG:HB3	2:E:4:PHE:CE1	2.54	0.43
1:D:724:ARG:HG2	1:D:725:LEU:HD12	2.01	0.43
1:A:741:TYR:HB3	1:A:743:PHE:CE1	2.54	0.42
4:A:1001:PCJ:H1	4:A:1001:PCJ:H12	1.99	0.42
1:D:268:THR:HB	1:D:278:THR:HG22	2.01	0.42
1:A:321:ARG:O	1:A:322:GLN:HG3	2.19	0.42
1:D:275:ASN:O	1:D:303:LYS:HA	2.19	0.42
1:D:605:PRO:HD2	1:D:640:PRO:HG3	2.01	0.42
1:D:823:VAL:CG2	1:D:824:ILE:N	2.83	0.42
1:D:276:ALA:O	1:D:303:LYS:N	2.35	0.42
1:D:398:PHE:CE1	1:D:876:ALA:HB2	2.53	0.42
1:D:652:THR:HG22	1:D:714:LEU:HD21	2.00	0.42
1:D:836:ARG:NH1	1:D:848:GLU:OE1	2.48	0.42
2:E:101:VAL:HG22	2:E:102:GLN:N	2.35	0.42
1:A:721:ASP:OD1	1:A:721:ASP:N	2.53	0.42
1:A:804:ARG:HB3	1:A:806:THR:HG22	2.00	0.42
1:A:828:VAL:CG1	1:A:829:PRO:CD	2.97	0.42
1:A:757:SER:HA	1:A:772:SER:O	2.19	0.42
2:E:137:ARG:O	2:E:141:LEU:HD13	2.19	0.42
1:A:188:VAL:HG22	1:A:210:LEU:HD13	2.02	0.42
1:A:269:ARG:HD3	1:A:896:GLY:CA	2.49	0.42
1:D:327:PRO:CG	1:D:899:GLY:HA2	2.50	0.42
1:D:834:LEU:HD12	1:D:834:LEU:O	2.19	0.42
2:E:155:ALA:HA	2:E:158:LYS:HE3	2.02	0.42
2:B:101:VAL:HG12	2:B:130:LEU:CD2	2.50	0.42
1:D:820:ASP:OD2	1:D:836:ARG:NH2	2.53	0.42
1:A:331:SER:OG	1:A:339:THR:HB	2.20	0.42
1:A:477:THR:HG22	1:A:533:ARG:HH22	1.85	0.42
1:D:224:VAL:HG12	1:D:225:GLN:N	2.34	0.42
1:D:282:ASN:N	1:D:296:THR:O	2.45	0.42
1:D:576:LYS:HE3	1:D:578:ASP:OD1	2.19	0.42
1:D:819:HIS:CE1	1:D:821:PHE:CD2	3.07	0.42
1:A:487:PRO:CD	1:A:512:ARG:HB3	2.40	0.42
1:A:328:PRO:HD3	4:A:1001:PCJ:C45	2.48	0.41
1:A:452:GLN:NE2	1:A:473:GLN:HB2	2.35	0.41
2:E:44:LYS:HD3	2:E:44:LYS:HA	1.95	0.41
1:A:694:PHE:CD1	1:A:694:PHE:N	2.89	0.41
2:B:101:VAL:CG2	2:B:102:GLN:N	2.84	0.41



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:330:PHE:CD1	1:A:330:PHE:N	2.87	0.41	
1:A:371:GLU:OE2	1:A:373:ARG:HD2	2.21	0.41	
1:D:617:ARG:HB3	2:E:4:PHE:CD1	2.56	0.41	
1:D:727:LEU:HD21	1:D:804:ARG:HH12	1.85	0.41	
1:D:775:PHE:CZ	1:D:777:TYR:HB2	2.54	0.41	
1:A:255:SER:HB3	1:A:256:GLU:H	1.72	0.41	
1:A:268:THR:HB	1:A:278:THR:HG22	2.02	0.41	
1:A:326:LEU:HB3	1:A:327:PRO:CD	2.50	0.41	
1:A:621:PHE:O	1:A:624:THR:OG1	2.32	0.41	
1:A:761:TRP:CZ2	1:A:766:SER:HA	2.55	0.41	
1:D:232:GLN:HA	1:D:252:ALA:O	2.20	0.41	
2:E:122:LEU:HD12	2:E:122:LEU:HA	1.76	0.41	
1:A:715:PRO:O	1:A:806:THR:OG1	2.38	0.41	
1:D:673:ARG:O	1:D:674:ILE:HD13	2.21	0.41	
1:D:859:CYS:O	1:D:860:TRP:HB3	2.21	0.41	
1:D:706:TYR:CG	1:D:710:ARG:NH1	2.89	0.41	
1:D:769:GLU:HG3	1:D:796:ASP:CB	2.51	0.41	
1:A:198:LEU:C	1:A:200:ASN:H	2.24	0.41	
1:A:592:ARG:NH1	1:A:724:ARG:HD2	2.36	0.41	
1:A:716:GLY:HA2	1:A:721:ASP:HB3	2.02	0.41	
1:D:327:PRO:HA	1:D:328:PRO:HD3	2.01	0.41	
1:D:765:THR:O	1:D:767:ARG:HG2	2.21	0.41	
1:D:850:PHE:CD1	1:D:850:PHE:C	2.93	0.41	
1:D:854:GLU:OE2	1:D:916:TYR:OH	2.38	0.41	
1:A:196:HIS:HB3	1:A:197:GLN:H	1.67	0.41	
1:A:401:TYR:CG	1:A:402:SER:N	2.89	0.41	
1:A:608:LYS:HE3	1:A:635:MET:CE	2.51	0.41	
2:B:62:GLN:NE2	2:B:76:PHE:CD2	2.89	0.41	
1:D:232:GLN:OE1	1:D:253:LYS:NZ	2.51	0.41	
1:D:592:ARG:HD2	1:D:724:ARG:HE	1.86	0.41	
1:D:722:LEU:HD13	1:D:728:ASP:OD2	2.21	0.41	
1:A:188:VAL:CG1	1:A:204:LEU:HD13	2.51	0.40	
1:A:279:LEU:HA	1:A:279:LEU:HD12	1.88	0.40	
1:A:232:GLN:HA	1:A:252:ALA:O	2.21	0.40	
1:A:592:ARG:O	1:A:592:ARG:HG2	2.21	0.40	
1:A:813:ASN:HB2	1:A:843:LYS:NZ	2.36	0.40	
1:D:701:ALA:HA	1:D:742:ALA:O	2.21	0.40	
1:A:384:ASN:O	1:A:408:TYR:HA	2.22	0.40	
1:D:511:VAL:HG13	1:D:513:PHE:CE2	2.56	0.40	
1:A:179:VAL:HG11	1:A:193:ALA:CB	2.51	0.40	
1:A:225:GLN:HB3	1:A:230:GLU:HB3	2.04	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:225:GLN:HG2	1:A:226:LEU:CD1	2.51	0.40	
4:A:1001:PCJ:O3	4:A:1001:PCJ:H452	2.21	0.40	
1:D:205:VAL:HG12	1:D:206:GLY:N	2.36	0.40	
1:D:567:THR:O	1:D:567:THR:HG22	2.21	0.40	
1:D:700:SER:O	1:D:743:PHE:HA	2.21	0.40	
1:D:789:VAL:HG13	1:D:821:PHE:HD1	1.86	0.40	
1:D:850:PHE:HB2	1:D:866:ASN:O	2.21	0.40	
1:A:218:VAL:O	1:A:236:ALA:HA	2.22	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	Perce	entiles
1	А	728/924~(79%)	679~(93%)	44 (6%)	5 (1%)	22	58
1	D	777/924~(84%)	719 (92%)	53~(7%)	5 (1%)	25	61
2	В	170/207~(82%)	164 (96%)	6 (4%)	0	100	100
2	Ε	170/207~(82%)	164 (96%)	5(3%)	1 (1%)	25	61
3	С	10/67~(15%)	10 (100%)	0	0	100	100
3	F	10/67~(15%)	10 (100%)	0	0	100	100
All	All	1865/2396~(78%)	1746 (94%)	108 (6%)	11 (1%)	25	61

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	487	PRO
1	D	121	LYS
1	А	487	PRO
1	D	198	LEU



Continued from previous page...

Mol	Chain	Res	Type
2	Е	40	ASN
1	А	206	GLY
1	А	526	ASP
1	А	195	LEU
1	А	257	ASN
1	D	132	PRO
1	D	913	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	Perce	ntiles
1	А	636/784~(81%)	625~(98%)	11 (2%)	60	84
1	D	678/784~(86%)	664 (98%)	14 (2%)	53	80
2	В	141/169~(83%)	137 (97%)	4 (3%)	43	75
2	Е	141/169~(83%)	138 (98%)	3(2%)	53	80
3	С	9/58~(16%)	9~(100%)	0	100	100
3	F	9/58~(16%)	8 (89%)	1 (11%)	6	23
All	All	1614/2022~(80%)	1581 (98%)	33 (2%)	55	81

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	201	ARG
1	А	227	ASP
1	А	244	HIS
1	А	260	ILE
1	А	330	PHE
1	А	388	LEU
1	А	486	LEU
1	А	525	ASP
1	А	604	LEU
1	А	605	PRO
1	А	758	ASP



7.6.1		- D	
Mol	Chain	Res	Type
2	В	9	LEU
2	В	97	ASN
2	В	109	GLU
2	В	148	GLU
1	D	130	ILE
1	D	146	MET
1	D	244	HIS
1	D	323	SER
1	D	419	ARG
1	D	446	SER
1	D	476	THR
1	D	484	ASP
1	D	517	LEU
1	D	604	LEU
1	D	629	THR
1	D	758	ASP
1	D	845	ARG
1	D	905	THR
2	Е	46	THR
2	Е	97	ASN
2	Е	129	ASP
3	F	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	452	GLN
2	В	62	GLN
2	В	98	GLN
1	D	412	ASN
1	D	830	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 monosaccharides 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).

Mal	Isl Trung Chain Dag I		ung Chain Dog Link		B	Bond lengths			Bond angles		
	туре	Unaim	res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
4	PCJ	D	1001	-	$60,\!61,\!61$	0.85	2 (3%)	59,65,65	1.46	9 (15%)	
4	PCJ	А	1001	-	60,61,61	2.03	11 (18%)	59,65,65	2.87	19 (32%)	

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
4	PCJ	D	1001	-	-	38/66/66/66	-
4	PCJ	А	1001	-	-	40/66/66/66	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	А	1001	PCJ	C66-N	8.68	1.52	1.34
4	А	1001	PCJ	O3-C26	6.73	1.53	1.33
4	D	1001	PCJ	O3-C26	4.04	1.45	1.33
4	D	1001	PCJ	O2-C46	3.83	1.45	1.34
4	А	1001	PCJ	CA-N	3.81	1.54	1.46
4	А	1001	PCJ	O2-C46	3.48	1.44	1.34
4	А	1001	PCJ	C25-C26	3.13	1.59	1.50
4	А	1001	PCJ	O28-C26	2.94	1.31	1.22
4	A	1001	PCJ	C45-C46	2.64	1.58	1.50
4	А	1001	PCJ	O3-C3	2.63	1.51	1.45



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	1001	PCJ	C65-C66	2.23	1.55	1.51
4	А	1001	PCJ	CB-SG	2.10	1.89	1.80
4	А	1001	PCJ	C24-C25	2.08	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1001	PCJ	C2-O2-C46	-11.36	89.82	117.79
4	А	1001	PCJ	C3-O3-C26	-9.57	81.66	117.12
4	D	1001	PCJ	CA-N-C66	5.62	131.21	122.92
4	А	1001	PCJ	O2-C46-C45	5.56	123.49	111.50
4	D	1001	PCJ	C65-C66-N	5.13	124.74	115.83
4	А	1001	PCJ	C44-C45-C46	-4.90	95.81	113.62
4	А	1001	PCJ	C63-C64-C65	-4.73	96.18	113.19
4	А	1001	PCJ	O2-C46-O47	-4.70	112.35	123.70
4	А	1001	PCJ	O3-C3-C2	4.22	120.72	108.43
4	А	1001	PCJ	C62-C61-C60	-4.03	93.98	114.42
4	А	1001	PCJ	C64-C65-C66	-3.60	103.15	113.26
4	А	1001	PCJ	C17-C16-C15	-3.58	96.27	114.42
4	А	1001	PCJ	C65-C66-N	3.48	121.86	115.83
4	D	1001	PCJ	O2-C46-C45	3.44	118.91	111.50
4	D	1001	PCJ	O67-C66-N	-3.32	117.36	122.95
4	А	1001	PCJ	C15-C14-C13	-2.78	100.31	114.42
4	D	1001	PCJ	C2-O2-C46	-2.74	111.05	117.79
4	А	1001	PCJ	O28-C26-C25	-2.69	113.23	123.73
4	А	1001	PCJ	C19-C18-C17	-2.62	101.14	114.42
4	А	1001	PCJ	O3-C26-C25	2.45	119.60	111.91
4	А	1001	PCJ	C-CA-N	2.33	114.81	109.60
4	А	1001	PCJ	C60-C59-C58	-2.31	102.70	114.42
4	D	1001	PCJ	C1-SG-CB	2.28	106.02	102.13
4	А	1001	PCJ	C11-C12-C13	-2.27	96.17	113.42
4	D	1001	PCJ	O67-C66-C65	-2.25	117.91	122.02
4	D	1001	PCJ	O3-C26-C25	2.22	118.89	111.91
4	А	1001	PCJ	O67-C66-C65	-2.14	118.11	122.02
4	D	1001	PCJ	C-CA-N	-2.08	104.94	109.60

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	1001	PCJ	C-CA-CB-SG
4	А	1001	PCJ	N-CA-CB-SG



Mol	Chain	Res	Type	Atoms	
4	А	1001	PCJ	CB-CA-N-C66	
4	D	1001	PCJ	C-CA-CB-SG	
4	D	1001	PCJ	N-CA-CB-SG	
4	D	1001	PCJ	SG-C1-C2-O2	
4	D	1001	PCJ	SG-C1-C2-C3	
4	D	1001	PCJ	C45-C46-O2-C2	
4	D	1001	PCJ	O28-C26-O3-C3	
4	А	1001	PCJ	O47-C46-O2-C2	
4	D	1001	PCJ	O47-C46-O2-C2	
4	D	1001	PCJ	C25-C26-O3-C3	
4	А	1001	PCJ	C45-C46-O2-C2	
4	D	1001	PCJ	C65-C66-N-CA	
4	А	1001	PCJ	C25-C26-O3-C3	
4	А	1001	PCJ	O28-C26-O3-C3	
4	А	1001	PCJ	C33-C34-C35-C36	
4	А	1001	PCJ	C65-C66-N-CA	
4	D	1001	PCJ	O67-C66-N-CA	
4	А	1001	PCJ	C35-C36-C37-C38	
4	А	1001	PCJ	O67-C66-N-CA	
4	А	1001	PCJ	C23-C24-C25-C26	
4	А	1001	PCJ	C43-C44-C45-C46	
4	D	1001	PCJ	O-C-CA-N	
4	А	1001	PCJ	C61-C62-C63-C64	
4	А	1001	PCJ	C36-C37-C38-C39	
4	А	1001	PCJ	C52-C53-C54-C55	
4	А	1001	PCJ	C54-C55-C56-C57	
4	А	1001	PCJ	C22-C23-C24-C25	
4	А	1001	PCJ	C41-C42-C43-C44	
4	D	1001	PCJ	C60-C61-C62-C63	
4	А	1001	PCJ	C42-C43-C44-C45	
4	D	1001	PCJ	C23-C24-C25-C26	
4	А	1001	PCJ	C32-C33-C34-C35	
4	А	1001	PCJ	C60-C61-C62-C63	
4	D	1001	PCJ	C19-C20-C21-C22	
4	D	1001	PCJ	C32-C33-C34-C35	
4	D	1001	PCJ	C42-C43-C44-C45	
4	А	1001	PCJ	C16-C17-C18-C19	
4	D	1001	PCJ	C53-C54-C55-C56	
4	А	1001	PCJ	C13-C14-C15-C16	
4	А	1001	PCJ	C14-C15-C16-C17	
4	А	1001	PCJ	C58-C59-C60-C61	
4	А	1001	PCJ	C56-C57-C58-C59	

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Mol	Chain	Res	Type	Atoms
4	D	1001	PCJ	C22-C23-C24-C25
4	А	1001	PCJ	C12-C13-C14-C15
4	А	1001	PCJ	C21-C22-C23-C24
4	D	1001	PCJ	C14-C15-C16-C17
4	D	1001	PCJ	C13-C14-C15-C16
4	D	1001	PCJ	C62-C63-C64-C65
4	А	1001	PCJ	C63-C64-C65-C66
4	А	1001	PCJ	C53-C54-C55-C56
4	D	1001	PCJ	C35-C36-C37-C38
4	D	1001	PCJ	C33-C34-C35-C36
4	D	1001	PCJ	C38-C39-C40-C41
4	А	1001	PCJ	C59-C60-C61-C62
4	А	1001	PCJ	C51-C52-C53-C54
4	D	1001	PCJ	C21-C22-C23-C24
4	D	1001	PCJ	C56-C57-C58-C59
4	А	1001	PCJ	C1-C2-C3-O3
4	А	1001	PCJ	C39-C40-C41-C42
4	D	1001	PCJ	C51-C52-C53-C54
4	А	1001	PCJ	C17-C18-C19-C20
4	А	1001	PCJ	O2-C2-C3-O3
4	D	1001	PCJ	C18-C19-C20-C21
4	D	1001	PCJ	C20-C21-C22-C23
4	D	1001	PCJ	CB-CA-N-C66
4	А	1001	PCJ	C18-C19-C20-C21
4	А	1001	PCJ	C19-C20-C21-C22
4	D	1001	PCJ	C41-C42-C43-C44
4	D	1001	PCJ	C57-C58-C59-C60
4	D	1001	PCJ	C44-C45-C46-O2
4	D	1001	PCJ	C54-C55-C56-C57
4	D	1001	PCJ	C34-C35-C36-C37
4	D	1001	PCJ	C40-C41-C42-C43
4	А	1001	PCJ	C31-C32-C33-C34
4	D	1001	PCJ	C44-C45-C46-O47
4	D	1001	PCJ	C58-C59-C60-C61

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There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1001	PCJ	4	0
4	А	1001	PCJ	26	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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, 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	736/924~(79%)	0.44	50 (6%) 17 9	49, 74, 122, 161	0
1	D	789/924~(85%)	0.45	62 (7%) 12 6	51, 83, 121, 147	0
2	В	172/207~(83%)	0.53	8 (4%) 31 18	55, 71, 116, 132	0
2	Е	172/207~(83%)	0.61	9 (5%) 27 16	58, 77, 116, 132	0
3	С	12/67~(17%)	1.44	3~(25%) 0 0	61, 67, 113, 120	0
3	F	12/67~(17%)	1.95	4 (33%) 0 0	65, 74, 116, 121	0
All	All	1893/2396~(79%)	0.48	136 (7%) 15 8	49, 77, 121, 161	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	174	THR	9.5
3	F	31	ALA	7.6
1	А	181	LEU	6.8
3	F	32	ASP	6.3
1	D	128	ALA	6.2
1	А	186	MET	5.9
3	С	31	ALA	5.3
1	D	230	GLU	5.2
1	А	289	ALA	5.1
1	А	191	ASP	5.0
1	А	527	GLY	4.9
1	D	228	ASN	4.8
3	С	32	ASP	4.8
1	А	228	ASN	4.7
3	С	30	PRO	4.7
1	A	906	GLU	4.6
1	D	183	GLN	4.5
1	А	188	VAL	4.4
2	В	164	LEU	4.4



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Mol	Chain	Res	Type	RSRZ
2	В	170	ALA	4.4
1	D	167	GLU	4.1
1	D	142	VAL	4.1
1	D	257	ASN	4.0
1	А	208	VAL	4.0
3	F	30	PRO	4.0
1	D	522	TYR	3.9
1	D	827	LEU	3.9
1	А	213	LYS	3.8
1	А	227	ASP	3.8
1	D	185	SER	3.8
2	Е	92	LEU	3.8
1	А	622	ALA	3.7
1	А	187	GLN	3.6
1	А	525	ASP	3.6
1	D	144	PRO	3.5
1	А	528	SER	3.5
1	D	258	ALA	3.4
1	D	226	LEU	3.4
1	D	129	GLU	3.4
1	А	202	GLY	3.3
1	А	593	ASP	3.3
1	D	621	PHE	3.3
1	А	781	VAL	3.2
1	А	623	GLY	3.2
1	D	141	PRO	3.2
1	D	186	MET	3.2
1	А	180	VAL	3.2
1	D	781	VAL	3.2
1	А	197	GLN	3.2
1	D	184	GLY	3.1
1	А	530	ARG	3.1
1	D	182	ARG	3.0
1	D	172	ILE	3.0
1	D	261	MET	2.9
1	D	181	LEU	2.9
1	D	624	THR	2.9
1	D	691	GLU	2.9
1	D	120	GLU	2.9
1	А	529	ILE	2.8
1	А	526	ASP	2.8
1	D	224	VAL	2.8



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Mol	Chain	Res	Type	RSRZ	
1	D	157	THR	2.8	
1	D	192	GLU	2.8	
1	А	190	GLY	2.8	
1	D	902	GLY	2.8	
1	А	855	TYR	2.8	
1	А	733 ASP		2.7	
1	D	215	MET	2.7	
1	D	529	ILE	2.7	
1	D	377	HIS	2.6	
1	А	727	LEU	2.6	
1	D	114	LEU	2.6	
1	А	726	ASN	2.6	
1	D	225	GLN	2.6	
1	D	870	LEU	2.6	
1	D	914	GLN	2.6	
2	В	16	LEU	2.5	
1	А	231	ALA	2.5	
1	А	199	GLU	2.5	
1	А	829	PRO	2.5	
1	А	831	TRP	2.5	
1	D	521	ILE	2.5	
1	D	625	PRO	2.5	
1	D	259	ILE	2.5	
1	D	913	ILE	2.4	
1	А	230	GLU	2.4	
1	А	256	GLU	2.4	
1	А	531	GLY	2.4	
2	Е	16	LEU	2.4	
2	Е	170	ALA	2.4	
1	D	127	LEU	2.4	
2	Е	88	GLY	2.4	
1	А	777	TYR	2.4	
2	Е	86	ILE	2.4	
1	D	199	GLU	2.4	
2	В	160	GLU	2.3	
1	А	200	ASN	2.3	
1	А	224	VAL	2.3	
1	А	621	PHE	2.3	
2	Е	87	VAL	2.3	
1	D	486	LEU	2.3	
2	В	92	LEU	2.3	
1	А	215	MET	2.2	



Mol	Chain	Res	Type	RSRZ
1	D	912	GLY	2.2
1	А	195	LEU	2.2
1	D	158	TYR	2.2
1	D	623	GLY	2.2
1	А	440	THR	2.2
2	В	64	THR	2.2
1	D	165	ARG	2.2
1	D	530	ARG	2.2
1	D	917	ARG	2.2
3	F	29	PRO	2.2
1	А	192	GLU	2.2
1	D	121	LYS	2.2
1	D	732	LEU	2.1
1	D	139	ILE	2.1
2	Е	79	THR	2.1
1	D	122	LEU	2.1
1	А	196	HIS	2.1
1	А	194	ASN	2.1
1	D	810	GLY	2.1
1	D	829	PRO	2.1
1	D	202	GLY	2.1
2	В	166	ALA	2.1
1	А	813	ASN	2.1
1	A	486	LEU	2.0
1	D	593	ASP	2.0
2	В	161	ALA	2.0
1	D	592	ARG	2.0
1	D	728	ASP	2.0
1	A	219	GLY	2.0
1	D	138	TYR	2.0
2	Е	64	THR	2.0
2	Е	172	ARG	2.0
1	D	524	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	PCJ	А	1001	62/62	0.78	0.44	44,60,69,99	0
4	PCJ	D	1001	62/62	0.83	0.38	41,60,72,80	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

