



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 PM GMT

PDB ID : 4KC5
Title : Crystal structure of the C-terminal part of RhiE from Burkholderia rhizoxinica
Authors : Zocher, G.; Heim, J.B.; Stehle, T.
Deposited on : 2013-04-24
Resolution : 2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

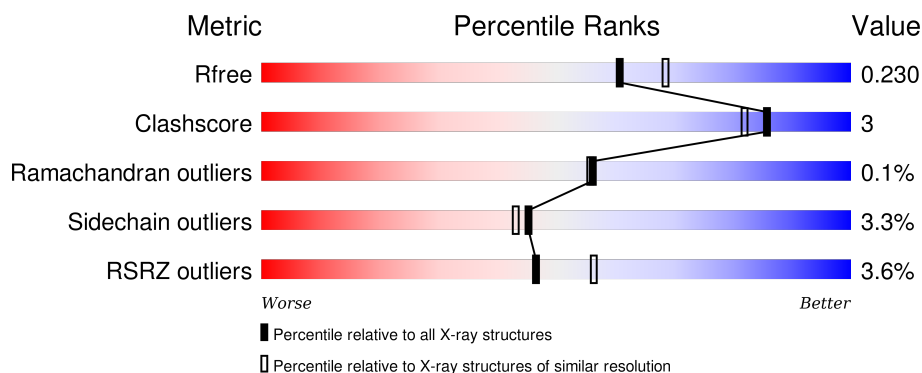
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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 $\leq 5\%$. 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	923	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	923	<div> <div>5%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	C	923	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	D	923	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	4001	-	-	-	X

2 Entry composition [i](#)

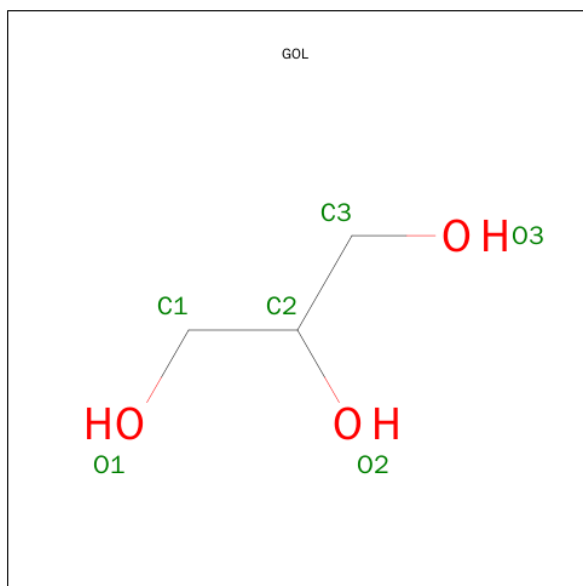
There are 3 unique types of molecules in this entry. The entry contains 29207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RhiE protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	914	Total	C	N	O	S	0	1	0
			7111	4506	1218	1356	31			
1	B	907	Total	C	N	O	S	0	0	0
			7035	4458	1205	1341	31			
1	C	901	Total	C	N	O	S	0	0	0
			6971	4419	1189	1332	31			
1	D	910	Total	C	N	O	S	0	1	0
			7068	4478	1215	1344	31			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

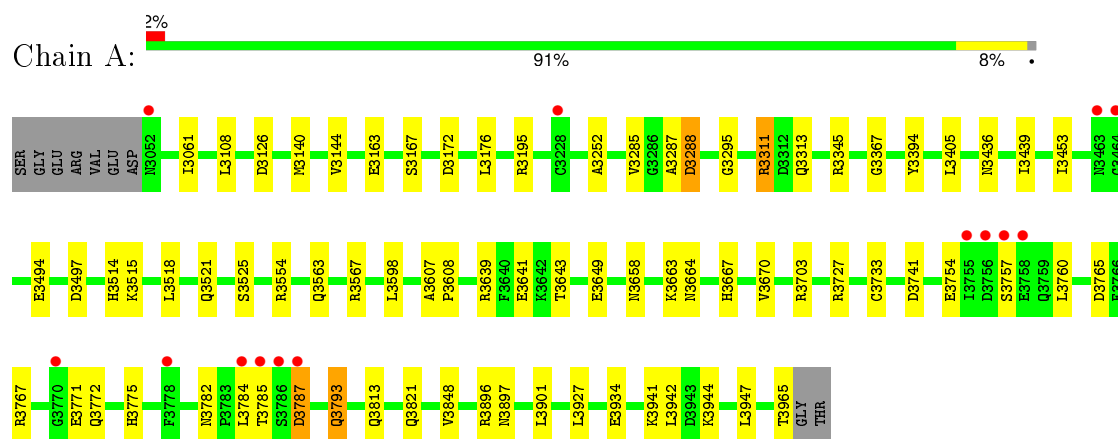
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	345	Total 345	O 345	0	0
3	B	207	Total 207	O 207	0	0
3	C	177	Total 177	O 177	0	0
3	D	287	Total 287	O 287	0	0

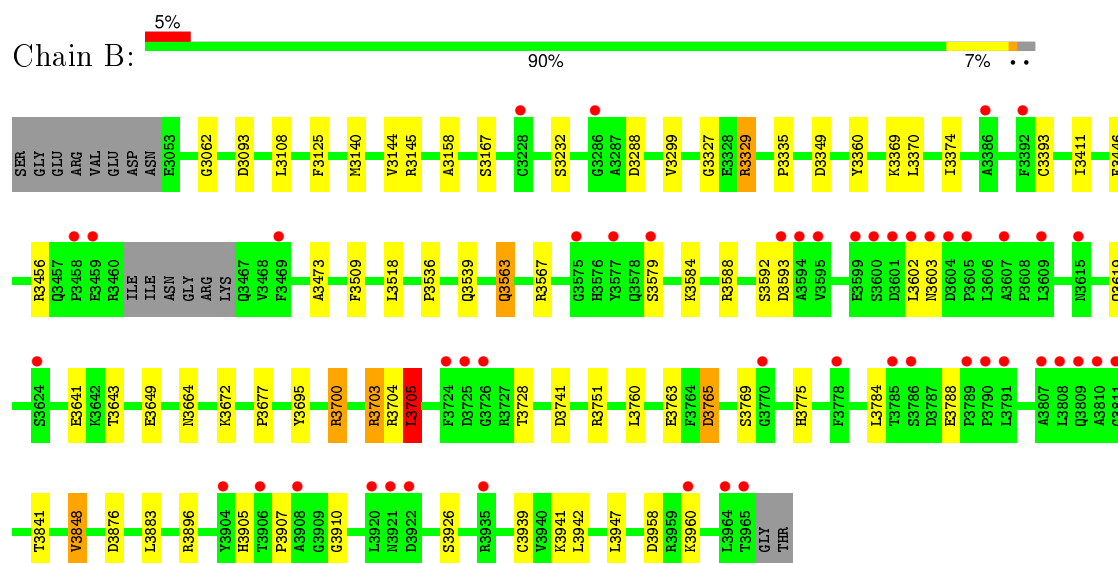
3 Residue-property plots [i](#)

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

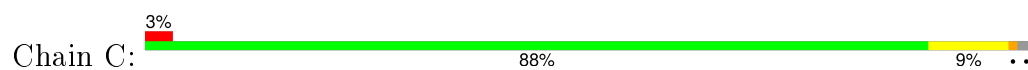
• Molecule 1: RhiE protein

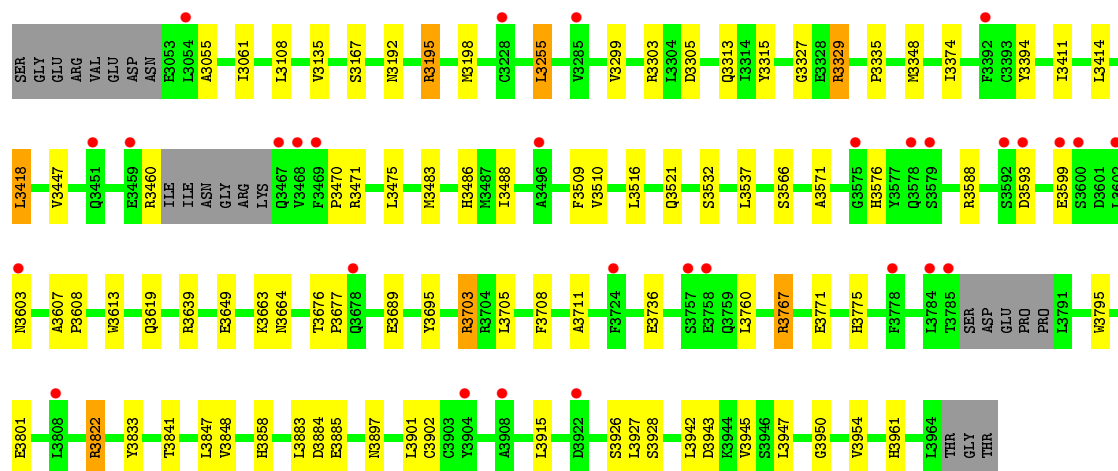


• Molecule 1: RhiE protein

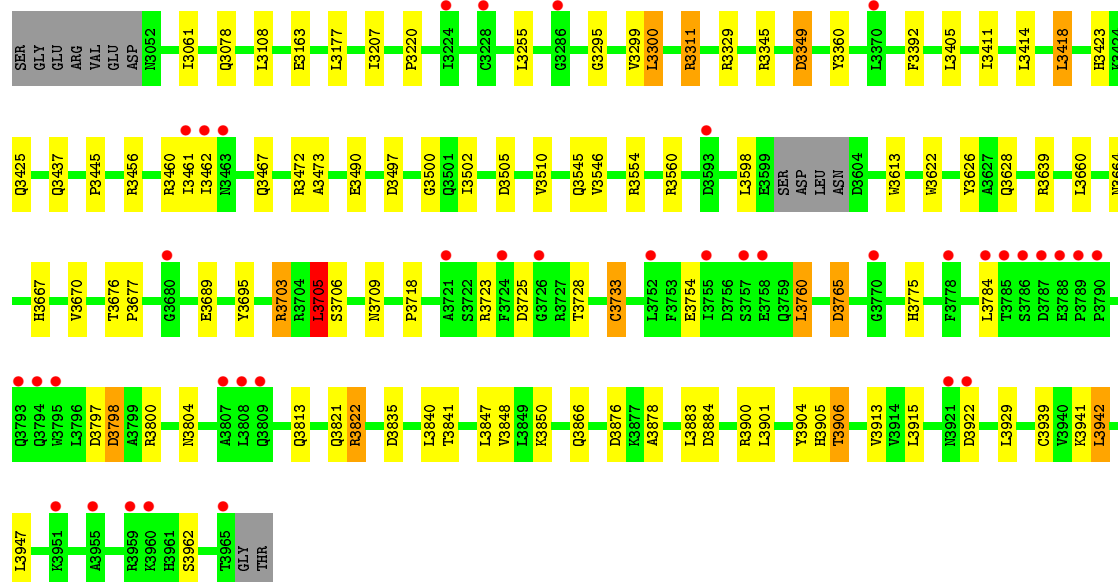
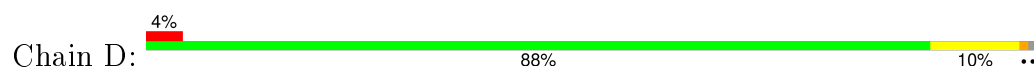


• Molecule 1: RhiE protein





• Molecule 1: RhiE protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.51Å 144.13Å 131.30Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	48.35 – 2.14 48.35 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.35-2.14) 99.2 (48.35-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.181 , 0.227 0.186 , 0.230	Depositor DCC
R_{free} test set	7585 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 252810 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29207	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL

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	0.79	4/7275 (0.1%)	0.84	8/9881 (0.1%)
1	B	0.66	0/7194	0.77	9/9774 (0.1%)
1	C	0.64	0/7127	0.74	5/9684 (0.1%)
1	D	0.76	3/7231 (0.0%)	0.83	11/9821 (0.1%)
All	All	0.72	7/28827 (0.0%)	0.80	33/39160 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3163	GLU	CG-CD	7.07	1.62	1.51
1	D	3163	GLU	CG-CD	6.07	1.61	1.51
1	A	3163	GLU	CB-CG	6.06	1.63	1.52
1	D	3939	CYS	CB-SG	-5.80	1.72	1.81
1	A	3649	GLU	CB-CG	5.50	1.62	1.52
1	A	3649	GLU	CG-CD	5.47	1.60	1.51
1	D	3733	CYS	CB-SG	-5.14	1.73	1.81

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3705	LEU	CA-CB-CG	9.89	138.04	115.30
1	D	3705	LEU	CA-CB-CG	8.57	135.01	115.30
1	D	3822	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	3703	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	D	3311	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	B	3703	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	B	3703	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	3311	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	3311	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	3311	ARG	NE-CZ-NH1	7.80	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3703	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	3703	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	3765	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	3093	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	3765	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	D	3822	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	3703	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	3456	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	3554	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	3703	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	3554	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	3703	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	3876	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	3163	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	C	3195	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	B	3741	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	3835	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	3741	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	3471	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	3195	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	D	3765	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	3876	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	3943	ASP	CB-CG-OD1	5.00	122.80	118.30

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	7111	0	6932	32	0
1	B	7035	0	6852	36	0
1	C	6971	0	6754	44	0
1	D	7068	0	6883	48	0
2	A	6	0	8	0	0
3	A	345	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	207	0	0	3	0
3	C	177	0	0	2	0
3	D	287	0	0	2	0
All	All	29207	0	27429	156	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 3.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3700:ARG:O	1:B:3704:ARG:NH2	2.17	0.78
1:A:3288:ASP:OD1	1:A:3288:ASP:C	2.30	0.70
1:A:3664:ASN:HD21	1:B:3664:ASN:HD21	1.41	0.67
1:C:3599:GLU:CB	3:C:4014:HOH:O	2.43	0.67
1:A:3765:ASP:OD1	1:A:3775:HIS:ND1	2.28	0.66
1:C:3847:LEU:HD11	1:C:3915:LEU:HD12	1.78	0.65
1:D:3472:ARG:HD3	1:D:3490:GLU:OE2	1.97	0.65
1:A:3311:ARG:NH2	1:A:3497:ASP:OD1	2.30	0.64
1:B:3751:ARG:NH2	1:B:3765:ASP:OD2	2.30	0.64
1:D:3840:LEU:HD11	1:D:3847:LEU:HD13	1.80	0.62
1:D:3295:GLY:HA3	1:D:3405:LEU:HD13	1.81	0.62
1:B:3728:THR:O	1:B:3784:LEU:HB2	1.99	0.62
1:A:3172:ASP:OD2	3:A:4297:HOH:O	2.16	0.61
1:B:3641:GLU:HG2	1:B:3643:THR:HG23	1.82	0.61
1:C:3885:GLU:OE2	1:C:3961:HIS:NE2	2.31	0.60
1:D:3639:ARG:HD2	3:D:4241:HOH:O	2.01	0.60
1:D:3311:ARG:NH2	1:D:3497:ASP:OD1	2.34	0.60
1:C:3509:PHE:CZ	1:C:3537:LEU:HD22	2.38	0.57
1:A:3785:THR:OG1	1:A:3787:ASP:HB2	2.05	0.57
1:D:3462:ILE:HD11	1:D:3467:GLN:OE1	2.03	0.57
1:A:3901:LEU:HD12	1:A:3942:LEU:HD22	1.85	0.57
1:C:3901:LEU:HD23	1:C:3902:CYS:N	2.20	0.57
1:A:3667:HIS:HB3	1:A:3670:VAL:HB	1.86	0.57
1:A:3607:ALA:HB3	1:A:3608:PRO:HD3	1.88	0.56
1:D:3061:ILE:HD11	1:D:3300:LEU:HD13	1.88	0.55
1:A:3436:ASN:HB3	1:A:3439:ILE:HD12	1.89	0.55
1:D:3345:ARG:O	1:D:3349:ASP:HB2	2.07	0.55
1:C:3695:TYR:HB3	1:C:3705:LEU:HD21	1.88	0.55
1:D:3705:LEU:HD13	1:D:3709:ASN:HD22	1.72	0.55
1:D:3822:ARG:HD3	1:D:3884:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3689:GLU:OE1	1:D:3703:ARG:HD3	2.07	0.54
1:D:3177:LEU:HD21	1:D:3207:ILE:HG22	1.90	0.54
1:C:3521:GLN:CG	1:C:3639:ARG:HD2	2.38	0.53
1:A:3287:ALA:HB1	1:A:3367:GLY:O	2.09	0.53
1:D:3728:THR:HG22	1:D:3784:LEU:HD22	1.91	0.52
1:D:3676:THR:HB	1:D:3677:PRO:HD2	1.91	0.52
1:D:3505:ASP:OD1	1:D:3560:ARG:NH1	2.43	0.52
1:A:3658:ASN:O	1:A:3663:LYS:HE2	2.09	0.52
1:D:3078:GLN:NE2	3:D:4083:HOH:O	2.30	0.52
1:C:3695:TYR:HB3	1:C:3705:LEU:CD2	2.40	0.51
1:C:3303:ARG:HD2	1:C:3305:ASP:OD1	2.11	0.51
1:B:3728:THR:O	1:B:3784:LEU:CB	2.59	0.50
1:B:3695:TYR:HB3	1:B:3705:LEU:HD22	1.93	0.50
1:D:3461:ILE:N	1:D:3461:ILE:HD12	2.27	0.50
1:C:3822:ARG:HD3	1:C:3884:ASP:OD2	2.12	0.50
1:D:3392:PHE:CE1	1:D:3445:PRO:HB3	2.47	0.50
1:B:3062:GLY:HA3	1:B:3158:ALA:HB2	1.93	0.49
1:C:3192:ASN:HA	1:C:3195:ARG:O	2.12	0.49
1:D:3765:ASP:OD1	1:D:3775:HIS:HA	2.12	0.49
1:A:3754:GLU:HG3	1:B:3677:PRO:HB2	1.94	0.49
1:C:3135:VAL:HG23	3:C:4121:HOH:O	2.12	0.49
1:A:3793:GLN:HE21	1:A:3793:GLN:HA	1.78	0.49
1:D:3723:ARG:NE	1:D:3754:GLU:OE2	2.45	0.49
1:D:3797:ASP:O	1:D:3800:ARG:N	2.45	0.49
1:B:3841:THR:HB	1:B:3848:VAL:HG13	1.95	0.49
1:D:3299:VAL:HG13	1:D:3411:ILE:HD11	1.93	0.49
1:D:3598:LEU:H	1:D:3598:LEU:HD23	1.77	0.49
1:D:3878:ALA:HB1	1:D:3915:LEU:HD11	1.93	0.49
1:C:3689:GLU:OE1	1:C:3703:ARG:HD3	2.13	0.49
1:C:3950:GLY:O	1:C:3954:VAL:HG23	2.13	0.48
1:D:3695:TYR:HB3	1:D:3705:LEU:HD22	1.94	0.48
1:B:3140:MET:HE3	1:B:3144:VAL:HG11	1.95	0.48
1:A:3295:GLY:HA3	1:A:3405:LEU:HD13	1.95	0.48
1:C:3942:LEU:HD21	1:C:3945:VAL:HG22	1.96	0.48
1:B:3536:PRO:HD2	1:B:3539:GLN:OE1	2.14	0.47
1:A:3521:GLN:HE21	1:A:3639:ARG:NH2	2.12	0.47
1:D:3510:VAL:HB	1:D:3613:TRP:CH2	2.49	0.47
1:D:3660:LEU:O	1:D:3664:ASN:HB2	2.15	0.47
1:B:3370:LEU:O	1:B:3374:ILE:HD12	2.14	0.47
1:D:3414:LEU:HG	1:D:3418:LEU:HD22	1.95	0.47
1:D:3866:GLN:O	1:D:3906:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3905:HIS:O	1:B:3939:CYS:HB3	2.15	0.47
1:A:3927:LEU:O	1:A:3944:LYS:HA	2.16	0.46
1:B:3299:VAL:HG13	1:B:3411:ILE:HD11	1.96	0.46
1:A:3518:LEU:HD11	1:A:3641:GLU:HB2	1.97	0.46
1:C:3676:THR:HB	1:C:3677:PRO:CD	2.46	0.46
1:C:3901:LEU:C	1:C:3901:LEU:HD23	2.36	0.46
1:D:3705:LEU:HD13	1:D:3709:ASN:ND2	2.30	0.46
1:D:3901:LEU:HD12	1:D:3942:LEU:HD22	1.97	0.45
1:A:3525:SER:HB2	1:A:3639:ARG:NH1	2.31	0.45
1:C:3394:TYR:CD1	1:C:3447:VAL:HG13	2.51	0.45
1:B:3958:ASP:OD1	1:B:3960:LYS:HB3	2.17	0.45
1:B:3703:ARG:NH2	3:B:4184:HOH:O	2.49	0.45
1:C:3255:LEU:N	1:C:3255:LEU:HD23	2.32	0.45
1:B:3509:PHE:HA	3:B:4093:HOH:O	2.16	0.45
1:C:3603:ASN:OD1	1:C:3603:ASN:N	2.49	0.45
1:C:3736:GLU:HG3	1:C:3775:HIS:CD2	2.51	0.45
1:C:3833:TYR:CE2	1:C:3858:HIS:HB2	2.52	0.45
1:C:3335:PRO:HG2	1:C:3374:ILE:HD13	1.99	0.44
1:B:3751:ARG:NH2	1:B:3765:ASP:CG	2.70	0.44
1:A:3126:ASP:OD2	1:A:3514[B]:HIS:CE1	2.70	0.44
1:D:3502:ILE:HD12	1:D:3626:TYR:CE2	2.52	0.44
1:A:3176:LEU:O	1:A:3252:ALA:HA	2.18	0.44
1:D:3676:THR:HB	1:D:3677:PRO:CD	2.47	0.44
1:D:3754:GLU:HA	1:D:3760:LEU:HD12	2.00	0.44
1:D:3706:SER:HB2	1:D:3876:ASP:OD2	2.18	0.44
1:B:3140:MET:CE	1:B:3144:VAL:CG1	2.95	0.44
1:B:3370:LEU:N	3:B:4094:HOH:O	2.35	0.44
1:B:3393:CYS:O	1:B:3446:PHE:HA	2.18	0.44
1:C:3483:MET:CE	1:D:3220:PRO:HA	2.48	0.43
1:C:3607:ALA:HB3	1:C:3608:PRO:HD3	2.00	0.43
1:B:3140:MET:HE3	1:B:3144:VAL:CG1	2.49	0.43
1:C:3767:ARG:NH1	1:C:3771:GLU:O	2.51	0.43
1:D:3667:HIS:HB3	1:D:3670:VAL:HB	2.00	0.43
1:A:3641:GLU:HG2	1:A:3643:THR:HG23	2.01	0.43
1:B:3167:SER:OG	1:B:3619:GLN:OE1	2.37	0.43
1:B:3751:ARG:NH1	1:B:3763:GLU:OE1	2.44	0.43
1:B:3518:LEU:HD11	1:B:3641:GLU:HB2	2.01	0.43
1:A:3563:GLN:HG2	1:A:3567:ARG:NH2	2.33	0.43
1:C:3847:LEU:C	1:C:3847:LEU:HD12	2.39	0.42
1:C:3795:TRP:CZ2	1:C:3928:SER:HB3	2.53	0.42
1:C:3571:ALA:O	1:C:3576:HIS:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3295:GLY:HA3	1:D:3405:LEU:CD1	2.49	0.42
1:C:3055:ALA:HA	1:C:3303:ARG:HD3	2.02	0.42
1:B:3907:PRO:HG3	1:B:3939:CYS:SG	2.59	0.42
1:D:3177:LEU:C	1:D:3177:LEU:HD12	2.40	0.42
1:D:3545:GLN:HB3	1:D:3622:TRP:CG	2.54	0.42
1:D:3904:TYR:O	1:D:3905:HIS:HB3	2.19	0.42
1:D:3848:VAL:HA	1:D:3913:VAL:O	2.19	0.42
1:D:3423:HIS:O	1:D:3425:GLN:HG3	2.19	0.42
1:C:3475:LEU:O	1:C:3486:HIS:HA	2.19	0.42
1:C:3315:TYR:HB3	1:C:3418:LEU:HG	2.02	0.41
1:C:3414:LEU:HG	1:C:3418:LEU:HD22	2.02	0.41
1:B:3563:GLN:H	1:B:3563:GLN:HE21	1.68	0.41
1:D:3500:GLY:HA2	1:D:3628:GLN:OE1	2.20	0.41
1:B:3125:PHE:CD1	1:B:3145:ARG:HB3	2.55	0.41
1:A:3641:GLU:OE1	1:A:3643:THR:HG21	2.21	0.41
1:C:3516:LEU:HD23	1:C:3516:LEU:HA	1.94	0.41
1:C:3510:VAL:HB	1:C:3613:TRP:CH2	2.55	0.41
1:C:3708:PHE:O	1:C:3711:ALA:HB3	2.20	0.41
1:C:3061:ILE:HA	1:C:3313:GLN:O	2.20	0.41
1:C:3521:GLN:HG2	1:C:3639:ARG:HD2	2.03	0.41
1:A:3767:ARG:NH1	1:A:3771:GLU:O	2.54	0.41
1:D:3360:TYR:O	1:D:3473:ALA:HA	2.21	0.41
1:A:3515:LYS:NZ	3:A:4316:HOH:O	2.54	0.41
1:A:3061:ILE:HA	1:A:3313:GLN:O	2.20	0.41
1:A:3664:ASN:HD21	1:B:3664:ASN:ND2	2.14	0.41
1:A:3525:SER:HB2	1:A:3639:ARG:HH11	1.86	0.41
1:C:3327:GLY:O	1:C:3329:ARG:HD3	2.21	0.41
1:A:3394:TYR:CE2	1:A:3453:ILE:HD11	2.56	0.41
1:B:3327:GLY:O	1:B:3329:ARG:HD3	2.20	0.41
1:A:3140:MET:HE3	1:A:3144:VAL:CG1	2.50	0.41
1:A:3641:GLU:OE1	1:A:3643:THR:CG2	2.69	0.40
1:C:3348:MET:HA	1:C:3488:ILE:HD13	2.03	0.40
1:B:3592:SER:O	1:B:3593:ASP:HB2	2.20	0.40
1:B:3765:ASP:OD1	1:B:3775:HIS:HD2	2.04	0.40
1:B:3335:PRO:HG2	1:B:3374:ILE:HD13	2.04	0.40
1:C:3167:SER:OG	1:C:3619:GLN:OE1	2.39	0.40
1:D:3797:ASP:O	1:D:3798:ASP:C	2.60	0.40
1:D:3841:THR:HB	1:D:3848:VAL:HG13	2.03	0.40
1:C:3299:VAL:HG13	1:C:3411:ILE:HD11	2.04	0.40
1:C:3676:THR:HB	1:C:3677:PRO:HD2	2.04	0.40
1:D:3929:LEU:C	1:D:3929:LEU:HD23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3841:THR:HB	1:C:3848:VAL:HG13	2.02	0.40
1:B:3288:ASP:OD1	1:B:3288:ASP:N	2.53	0.40
1:B:3360:TYR:O	1:B:3473:ALA:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	913/923 (99%)	898 (98%)	14 (2%)	1 (0%)	56	56
1	B	903/923 (98%)	880 (98%)	22 (2%)	1 (0%)	56	56
1	C	895/923 (97%)	874 (98%)	21 (2%)	0	100	100
1	D	907/923 (98%)	873 (96%)	32 (4%)	2 (0%)	52	50
All	All	3618/3692 (98%)	3525 (97%)	89 (2%)	4 (0%)	56	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3798	ASP
1	A	3757	SER
1	B	3910	GLY
1	D	3900	ARG

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	762/778 (98%)	738 (97%)	24 (3%)	47	46
1	B	754/778 (97%)	727 (96%)	27 (4%)	42	39
1	C	742/778 (95%)	719 (97%)	23 (3%)	47	46
1	D	755/778 (97%)	730 (97%)	25 (3%)	45	43
All	All	3013/3112 (97%)	2914 (97%)	99 (3%)	45	43

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3108	LEU
1	A	3167	SER
1	A	3285	VAL
1	A	3288	ASP
1	A	3345	ARG
1	A	3494	GLU
1	A	3598	LEU
1	A	3727	ARG
1	A	3733	CYS
1	A	3760	LEU
1	A	3772	GLN
1	A	3782	ASN
1	A	3784	LEU
1	A	3787	ASP
1	A	3793	GLN
1	A	3813	GLN
1	A	3821	GLN
1	A	3848	VAL
1	A	3896	ARG
1	A	3897	ASN
1	A	3934	GLU
1	A	3941	LYS
1	A	3947	LEU
1	A	3965	THR
1	B	3108	LEU
1	B	3232	SER
1	B	3329	ARG
1	B	3349	ASP
1	B	3369	LYS
1	B	3456	ARG
1	B	3563	GLN

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Mol	Chain	Res	Type
1	B	3567	ARG
1	B	3579	SER
1	B	3584	LYS
1	B	3588	ARG
1	B	3602	LEU
1	B	3603	ASN
1	B	3649	GLU
1	B	3672	LYS
1	B	3700	ARG
1	B	3705	LEU
1	B	3760	LEU
1	B	3769	SER
1	B	3788	GLU
1	B	3848	VAL
1	B	3883	LEU
1	B	3896	ARG
1	B	3926	SER
1	B	3941	LYS
1	B	3942	LEU
1	B	3947	LEU
1	C	3108	LEU
1	C	3198	MET
1	C	3255	LEU
1	C	3329	ARG
1	C	3418	LEU
1	C	3460	ARG
1	C	3470	PRO
1	C	3532	SER
1	C	3566	SER
1	C	3588	ARG
1	C	3593	ASP
1	C	3649	GLU
1	C	3663	LYS
1	C	3664	ASN
1	C	3760	LEU
1	C	3767	ARG
1	C	3801	GLU
1	C	3822	ARG
1	C	3883	LEU
1	C	3897	ASN
1	C	3926	SER
1	C	3927	LEU

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Mol	Chain	Res	Type
1	C	3947	LEU
1	D	3108	LEU
1	D	3255	LEU
1	D	3300	LEU
1	D	3329	ARG
1	D	3349	ASP
1	D	3418	LEU
1	D	3437	GLN
1	D	3460	ARG
1	D	3546	VAL
1	D	3705	LEU
1	D	3718	PRO
1	D	3725	ASP
1	D	3733	CYS
1	D	3760	LEU
1	D	3804	ASN
1	D	3813	GLN
1	D	3821	GLN
1	D	3850	LYS
1	D	3883	LEU
1	D	3906	THR
1	D	3922	ASP
1	D	3941	LYS
1	D	3942	LEU
1	D	3947	LEU
1	D	3962	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3521	GLN
1	A	3612	GLN
1	A	3793	GLN
1	A	3794	GLN
1	B	3313	GLN
1	B	3563	GLN
1	B	3612	GLN
1	B	3615	ASN
1	B	3664	ASN
1	B	3709	ASN
1	B	3775	HIS
1	B	3952	GLN

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Mol	Chain	Res	Type
1	C	3772	GLN
1	D	3149	GLN
1	D	3266	ASN
1	D	3709	ASN
1	D	3905	HIS

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](#)

1 ligand is 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	GOL	A	4001	-	5,5,5	0.79	0	5,5,5	0.94	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	GOL	A	4001	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	914/923 (99%)	-0.06	14 (1%)	76	82	21, 35, 62, 89	0
1	B	907/923 (98%)	0.23	49 (5%)	29	38	27, 48, 79, 118	0
1	C	901/923 (97%)	0.13	30 (3%)	50	59	29, 48, 77, 109	0
1	D	910/923 (98%)	0.08	38 (4%)	40	49	23, 39, 76, 113	0
All	All	3632/3692 (98%)	0.10	131 (3%)	46	56	21, 42, 76, 118	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3602	LEU	9.5
1	B	3600	SER	6.4
1	D	3785	THR	6.1
1	C	3602	LEU	5.7
1	B	3603	ASN	5.6
1	D	3787	ASP	5.4
1	D	3786	SER	5.3
1	B	3599	GLU	5.2
1	B	3785	THR	5.0
1	A	3787	ASP	4.8
1	D	3755	ILE	4.8
1	D	3790	PRO	4.8
1	B	3786	SER	4.8
1	C	3603	ASN	4.5
1	B	3965	THR	4.5
1	D	3757	SER	4.5
1	D	3784	LEU	4.4
1	A	3757	SER	4.4
1	B	3960	LYS	4.4
1	D	3462	ILE	4.3
1	B	3790	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	3463	ASN	4.2
1	B	3808	LEU	4.2
1	B	3789	PRO	4.0
1	B	3605	PRO	3.8
1	C	3908	ALA	3.8
1	C	3600	SER	3.8
1	B	3809	GLN	3.7
1	B	3922	ASP	3.6
1	C	3468	VAL	3.5
1	D	3793	GLN	3.5
1	B	3726	GLY	3.4
1	A	3755	ILE	3.4
1	D	3593	ASP	3.3
1	D	3960	LYS	3.2
1	B	3807	ALA	3.2
1	C	3459	GLU	3.1
1	B	3920	LEU	3.1
1	C	3467	GLN	3.1
1	D	3778	PHE	3.0
1	A	3464	GLY	3.0
1	C	3496	ALA	3.0
1	D	3951	LYS	3.0
1	B	3459	GLU	3.0
1	D	3788	GLU	3.0
1	A	3785	THR	2.9
1	D	3770	GLY	2.9
1	D	3789	PRO	2.9
1	D	3724	PHE	2.8
1	B	3725	ASP	2.8
1	D	3809	GLN	2.8
1	B	3904	TYR	2.8
1	B	3615	ASN	2.8
1	D	3922	ASP	2.7
1	A	3770	GLY	2.7
1	B	3593	ASP	2.7
1	B	3607	ALA	2.7
1	B	3392	PHE	2.7
1	C	3808	LEU	2.7
1	C	3904	TYR	2.7
1	C	3778	PHE	2.7
1	B	3286	GLY	2.7
1	B	3811	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	3758	GLU	2.6
1	B	3595	VAL	2.6
1	D	3721	ALA	2.6
1	D	3726	GLY	2.6
1	C	3922	ASP	2.6
1	A	3786	SER	2.5
1	A	3463	ASN	2.5
1	A	3778	PHE	2.5
1	B	3386	ALA	2.5
1	B	3609	LEU	2.5
1	B	3458	PRO	2.5
1	B	3791	LEU	2.5
1	B	3624	SER	2.5
1	D	3959	ARG	2.5
1	B	3778	PHE	2.5
1	B	3921	ASN	2.5
1	A	3758	GLU	2.4
1	D	3370	LEU	2.4
1	B	3724	PHE	2.4
1	B	3906	THR	2.4
1	C	3784	LEU	2.4
1	B	3601	ASP	2.4
1	C	3757	SER	2.4
1	C	3599	GLU	2.3
1	B	3228	CYS	2.3
1	B	3964	LEU	2.3
1	A	3052	ASN	2.3
1	B	3935	ARG	2.3
1	C	3578	GLN	2.3
1	C	3451	GLN	2.3
1	C	3469	PHE	2.3
1	B	3575	GLY	2.3
1	D	3795	TRP	2.3
1	D	3461	ILE	2.3
1	C	3785	THR	2.3
1	B	3604	ASP	2.3
1	C	3592	SER	2.2
1	D	3228	CYS	2.2
1	C	3724	PHE	2.2
1	B	3810	ALA	2.2
1	C	3758	GLU	2.2
1	D	3955	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3908	ALA	2.2
1	B	3579	SER	2.2
1	B	3770	GLY	2.2
1	C	3593	ASP	2.2
1	D	3224	ILE	2.2
1	A	3228	CYS	2.1
1	C	3228	CYS	2.1
1	D	3921	ASN	2.1
1	D	3794	GLN	2.1
1	D	3807	ALA	2.1
1	C	3579	SER	2.1
1	D	3965	THR	2.1
1	D	3808	LEU	2.1
1	C	3678	GLN	2.1
1	C	3285	VAL	2.1
1	C	3575	GLY	2.1
1	C	3054	LEU	2.1
1	A	3756	ASP	2.1
1	B	3577	TYR	2.1
1	A	3784	LEU	2.1
1	B	3469	PHE	2.1
1	D	3752	LEU	2.0
1	D	3680	GLY	2.0
1	D	3286	GLY	2.0
1	B	3594	ALA	2.0
1	C	3392	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	A	4001	6/6	0.95	0.14	6.01	31,34,37,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.