



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:43 am GMT

PDB ID : 3N96
Title : Crystal structure of human CRFR2 alpha extracellular domain in complex with Urocortin 1
Authors : Pal, K.; Swaminathan, K.; Pioszak, A.A.; Xu, H.E.
Deposited on : 2010-05-28
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

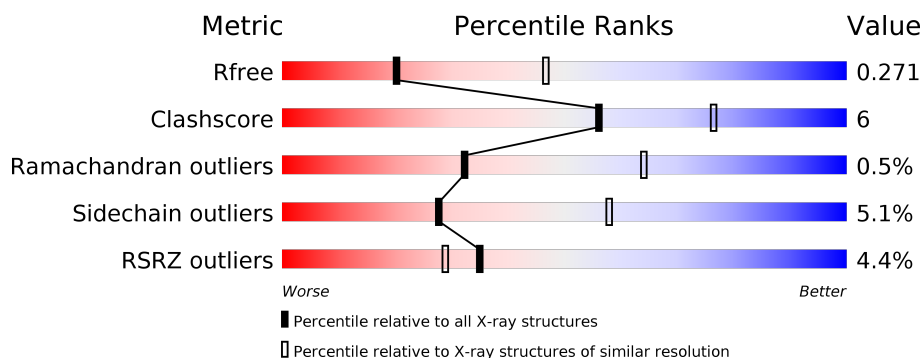
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	482	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 82%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 82% 15% .. </div> </div>
1	B	482	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 85%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 85% 12% .. </div> </div>
1	C	482	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 14%, green 82%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 6% 82% 14% .. </div> </div>
1	D	482	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 14%, green 82%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 5% 82% 14% .. </div> </div>
2	E	17	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 12%, orange 1%, yellow 18%, green 82%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 12% 82% 18% </div> </div>
2	F	17	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 6%, green 94%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 6% 94% 6% </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	17	<div><div></div><div></div><div></div><div></div><div></div></div> <div>59%65%12%12%12%</div>
2	H	17	<div><div></div><div></div><div></div><div></div><div></div></div> <div>35%47%18%35%</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15249 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 Maltose binding protein-CRFR2 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3667	2351	597	707	12			
1	B	471	Total	C	N	O	S	0	0	0
			3651	2341	595	703	12			
1	C	467	Total	C	N	O	S	0	0	0
			3623	2325	591	695	12			
1	D	468	Total	C	N	O	S	0	0	0
			3631	2329	592	698	12			

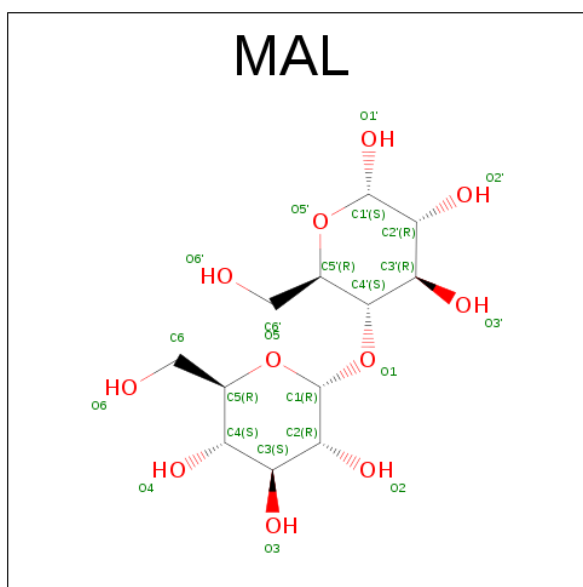
- Molecule 2 is a protein called Urocortin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	0	0	1
			137	81	29	27			
2	F	17	Total	C	N	O	0	0	1
			137	81	29	27			
2	G	15	Total	C	N	O	0	0	1
			122	73	26	23			
2	H	11	Total	C	N	O	0	0	1
			86	53	16	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	NH2	-	AMIDATION	UNP P55089
F	42	NH2	-	AMIDATION	UNP P55089
G	42	NH2	-	AMIDATION	UNP P55089
H	42	NH2	-	AMIDATION	UNP P55089

- Molecule 3 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

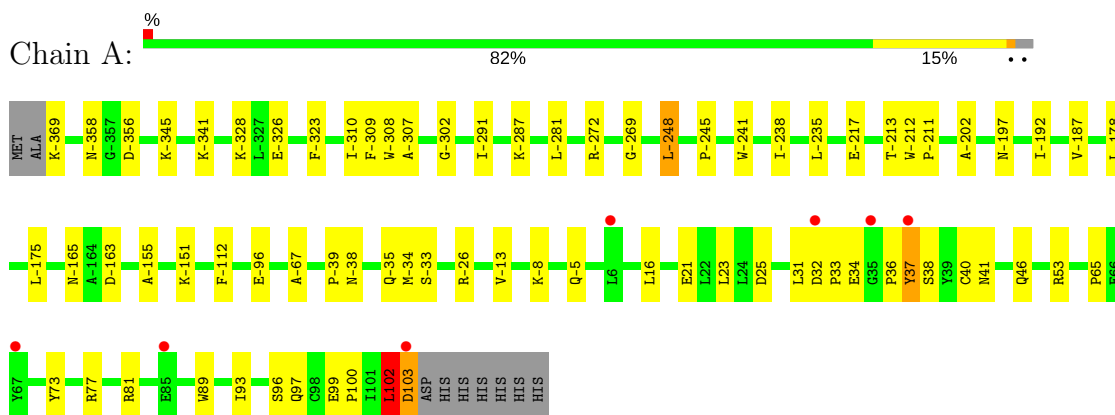
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	33	Total	O	0	0
			33	33		
4	C	24	Total	O	0	0
			24	24		
4	D	18	Total	O	0	0
			18	18		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		

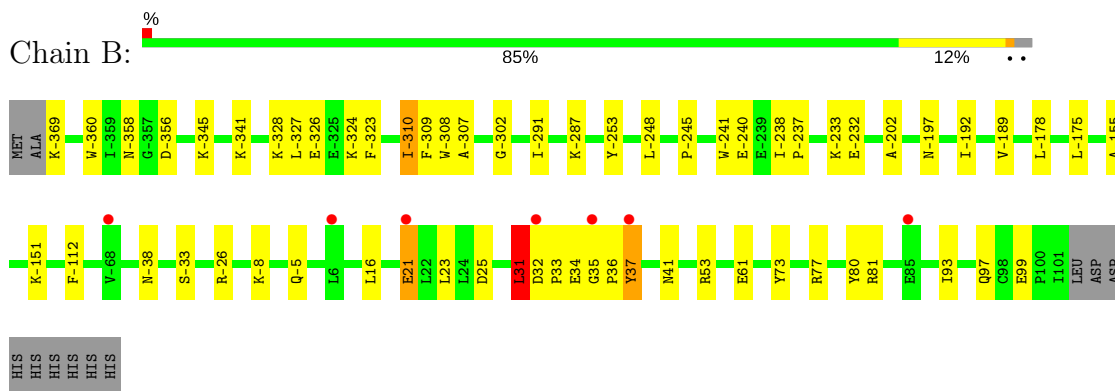
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

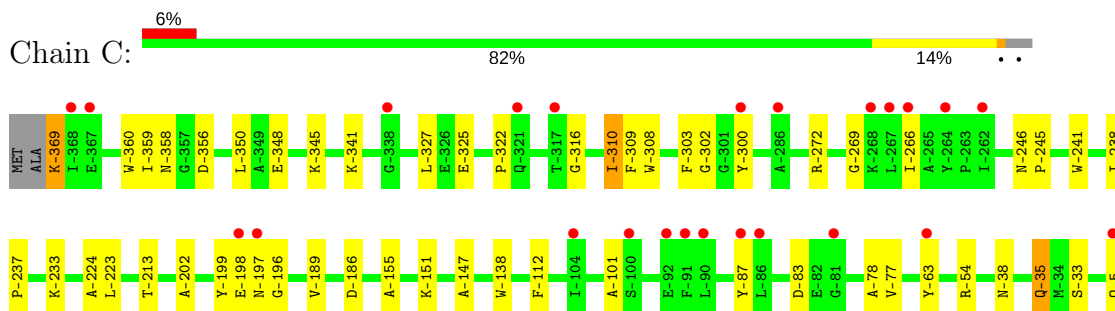
- Molecule 1: Maltose binding protein-CRFR2 alpha

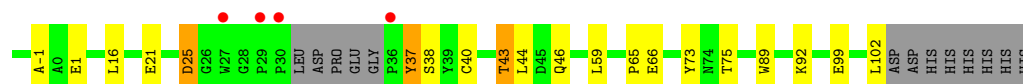


- Molecule 1: Maltose binding protein-CRFR2 alpha

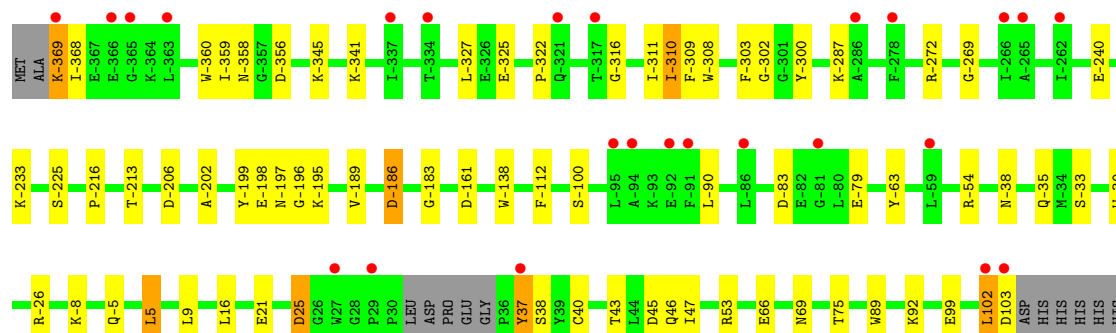
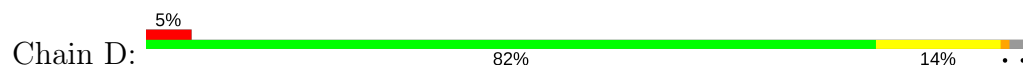


- Molecule 1: Maltose binding protein-CRFR2 alpha



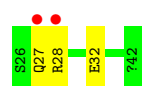
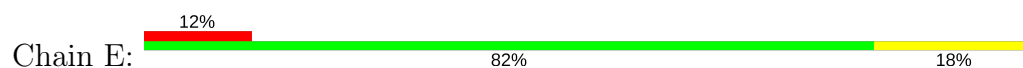


• Molecule 1: Maltose binding protein-CRFR2 alpha



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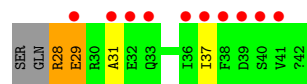
• Molecule 2: Urocortin



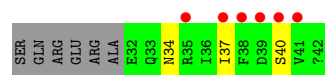
• Molecule 2: Urocortin



• Molecule 2: Urocortin



• Molecule 2: Urocortin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.06Å 211.55Å 107.84Å 90.00° 104.37° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 35.26 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.75) 94.3 (35.26-2.72)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.235 , 0.273 0.232 , 0.271	Depositor DCC
R_{free} test set	2923 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAL, NH2

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	0.86	2/3759 (0.1%)	0.82	3/5115 (0.1%)
1	B	0.83	0/3743	0.78	4/5093 (0.1%)
1	C	0.79	0/3713	0.76	0/5049
1	D	0.84	0/3721	0.82	5/5060 (0.1%)
2	E	0.66	0/136	0.78	0/180
2	F	0.64	0/136	0.75	0/180
2	G	0.56	0/121	0.67	0/160
2	H	0.54	0/85	0.54	0/113
All	All	0.83	2/15414 (0.0%)	0.80	12/20950 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-217	GLU	CG-CD	6.07	1.61	1.51
1	A	-96	GLU	CD-OE2	5.08	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-26	ARG	NE-CZ-NH1	7.08	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-26	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	D	69	ASN	N-CA-C	6.70	129.08	111.00
1	A	-248	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	B	31	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	102	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	-26	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	D	-161	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	45	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	-186	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	35	GLY	N-CA-C	-5.11	100.33	113.10
1	B	-248	LEU	CB-CG-CD1	-5.09	102.34	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	37	TYR	Peptide
1	D	37	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3667	0	3585	46	0
1	B	3651	0	3570	44	0
1	C	3623	0	3550	56	0
1	D	3631	0	3554	45	0
2	E	137	0	131	3	0
2	F	137	0	131	2	0
2	G	122	0	118	5	0
2	H	86	0	81	6	0
3	A	23	0	22	0	0
3	B	23	0	22	0	0
3	C	23	0	22	0	0
3	D	23	0	22	0	0
4	A	23	0	0	0	0
4	B	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	24	0	0	15	0
4	D	18	0	0	1	0
4	E	1	0	0	2	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
All	All	15249	0	14808	173	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 6.

All (173) 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:C:-350:LEU:HA	4:C:125:HOH:O	1.46	1.15
1:B:37:TYR:CE2	1:C:-189:VAL:O	2.06	1.09
1:C:-77:VAL:CG2	4:C:125:HOH:O	2.02	1.04
1:B:37:TYR:CZ	1:C:-189:VAL:O	2.12	1.01
1:C:-348:GLU:HB2	4:C:131:HOH:O	1.63	0.99
1:A:37:TYR:CE2	1:D:-189:VAL:O	2.19	0.95
1:B:37:TYR:OH	1:C:-5:GLN:OE1	1.89	0.91
1:C:-348:GLU:CB	4:C:131:HOH:O	2.22	0.87
2:E:32:GLU:HB2	4:E:50:HOH:O	1.75	0.85
1:C:-77:VAL:HG22	4:C:125:HOH:O	1.68	0.84
1:A:37:TYR:CZ	1:D:-189:VAL:O	2.31	0.84
2:E:28:ARG:O	4:E:50:HOH:O	1.95	0.82
1:B:-302:GLY:HA3	1:B:-38:ASN:O	1.80	0.81
1:A:102:LEU:O	1:A:103:ASP:HB3	1.80	0.81
1:B:-328:LYS:NZ	2:H:37:ILE:HD11	1.96	0.80
1:B:-328:LYS:HZ1	2:H:37:ILE:HD11	1.45	0.79
1:A:31:LEU:HG	1:A:32:ASP:H	1.48	0.77
1:A:-328:LYS:NZ	2:G:37:ILE:HD11	1.99	0.77
1:C:-302:GLY:HA3	1:C:-38:ASN:O	1.84	0.77
1:D:-302:GLY:HA3	1:D:-38:ASN:O	1.87	0.75
1:C:-224:ALA:O	4:C:130:HOH:O	2.07	0.71
1:A:-302:GLY:HA3	1:A:-38:ASN:O	1.92	0.69
1:A:-328:LYS:HZ1	2:G:37:ILE:HD11	1.59	0.68
1:D:40:CYS:HB3	1:D:89:TRP:CE2	2.30	0.67
1:C:-101:ALA:HB2	4:C:115:HOH:O	1.95	0.67
1:B:-326:GLU:N	1:B:-326:GLU:OE1	2.26	0.66
1:A:37:TYR:OH	1:D:-5:GLN:OE1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-8:LYS:O	1:B:-5:GLN:HB3	1.97	0.64
1:A:-178:LEU:HD12	1:A:-175:LEU:HD23	1.83	0.61
1:B:37:TYR:OH	1:C:-189:VAL:HG12	2.00	0.61
1:A:41:ASN:HA	1:A:53:ARG:HG3	1.82	0.61
1:C:-87:TYR:OH	4:C:133:HOH:O	2.11	0.61
1:B:41:ASN:ND2	4:B:130:HOH:O	2.31	0.60
1:D:37:TYR:O	1:D:37:TYR:CD2	2.54	0.60
1:D:40:CYS:HB3	1:D:89:TRP:NE1	2.17	0.60
1:B:32:ASP:C	1:B:34:GLU:H	2.05	0.60
1:D:-8:LYS:O	1:D:-5:GLN:HB3	2.01	0.59
1:A:32:ASP:C	1:A:34:GLU:H	2.06	0.59
1:D:-83:ASP:OD1	1:D:-63:TYR:HB2	2.02	0.59
1:D:-195:LYS:HB2	4:D:112:HOH:O	2.02	0.59
1:A:37:TYR:HE1	1:D:-186:ASP:H	1.50	0.59
1:C:40:CYS:HB3	1:C:89:TRP:CE2	2.38	0.58
1:C:-1:ALA:O	1:C:1:GLU:N	2.37	0.58
1:C:37:TYR:O	1:C:37:TYR:CD2	2.57	0.58
1:C:-78:ALA:HB1	4:C:131:HOH:O	2.04	0.57
1:D:-138:TRP:CH2	1:D:-54:ARG:HB3	2.40	0.57
1:B:37:TYR:HD2	1:B:37:TYR:O	1.88	0.57
1:C:102:LEU:HB3	2:E:28:ARG:HH11	1.68	0.57
1:A:100:PRO:HG2	2:G:31:ALA:HB1	1.86	0.57
1:A:-326:GLU:N	1:A:-326:GLU:OE1	2.33	0.56
1:D:-322:PRO:HG3	1:D:-300:TYR:CE1	2.39	0.56
1:D:37:TYR:HD2	1:D:37:TYR:O	1.87	0.56
1:B:-192:ILE:CD1	1:C:38:SER:HB2	2.35	0.56
1:D:-360:TRP:HB3	1:D:-327:LEU:HD11	1.88	0.56
1:B:73:TYR:OH	2:H:34:ASN:ND2	2.38	0.56
1:B:-324:LYS:NZ	2:H:40:SER:OG	2.36	0.56
1:D:-199:TYR:OH	1:D:-196:GLY:HA2	2.06	0.55
1:C:37:TYR:O	1:C:37:TYR:HD2	1.88	0.55
1:A:31:LEU:HG	1:A:32:ASP:N	2.21	0.54
1:B:-178:LEU:HD12	1:B:-175:LEU:HD23	1.90	0.54
1:D:47:ILE:HD13	2:F:38:PHE:CD1	2.43	0.54
1:A:-165:ASN:OD1	1:A:-163:ASP:HB2	2.08	0.53
1:C:-316:GLY:HA2	4:C:115:HOH:O	2.08	0.53
1:C:37:TYR:HA	4:C:132:HOH:O	2.08	0.53
1:A:37:TYR:OH	1:D:-189:VAL:HG12	2.09	0.53
1:B:-358:ASN:ND2	1:B:-356:ASP:OD1	2.42	0.53
1:A:77:ARG:HD3	1:A:97:GLN:O	2.09	0.52
1:D:-79:GLU:HA	1:D:-63:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-310:ILE:HG12	1:C:-309:PHE:N	2.23	0.52
1:A:-328:LYS:HZ2	2:G:37:ILE:HD11	1.71	0.52
1:A:37:TYR:HH	1:D:-5:GLN:CD	2.07	0.52
1:D:-369:LYS:HA	1:D:-316:GLY:O	2.09	0.52
1:C:-83:ASP:OD1	1:C:-63:TYR:HB2	2.10	0.52
1:C:-138:TRP:CH2	1:C:-54:ARG:HB3	2.44	0.52
1:C:-322:PRO:HG3	1:C:-300:TYR:CE1	2.44	0.51
1:C:-360:TRP:HB3	1:C:-327:LEU:HD11	1.93	0.51
1:B:73:TYR:OH	2:H:34:ASN:CB	2.59	0.51
1:C:-223:LEU:HA	4:C:130:HOH:O	2.10	0.51
1:C:-77:VAL:HG23	4:C:125:HOH:O	1.89	0.50
1:C:-224:ALA:C	4:C:130:HOH:O	2.48	0.50
1:D:47:ILE:HD13	2:F:38:PHE:CE1	2.46	0.50
1:B:-192:ILE:HD12	1:C:38:SER:HB2	1.94	0.50
1:C:-325:GLU:O	1:C:-322:PRO:HD2	2.12	0.49
1:D:-311:ILE:HD13	1:D:-90:LEU:HD11	1.95	0.49
1:B:37:TYR:HE1	1:C:-186:ASP:H	1.60	0.49
1:A:37:TYR:HD2	1:A:37:TYR:O	1.97	0.48
1:D:-359:ILE:HG13	1:D:-309:PHE:CB	2.44	0.48
1:A:-192:ILE:CD1	1:D:38:SER:HB2	2.44	0.48
1:D:40:CYS:O	1:D:53:ARG:HA	2.13	0.48
1:A:73:TYR:CE2	1:A:100:PRO:HG3	2.49	0.48
1:B:37:TYR:CD2	1:B:37:TYR:O	2.66	0.48
1:A:-39:PRO:HG2	1:A:-34:MET:SD	2.54	0.47
1:C:-272:ARG:HD3	1:C:-269:GLY:HA2	1.95	0.47
1:C:-369:LYS:HA	1:C:-316:GLY:O	2.14	0.47
1:D:-240:GLU:OE1	1:D:-240:GLU:N	2.38	0.47
2:G:28:ARG:HB2	2:G:29:GLU:HG3	1.96	0.47
1:D:-186:ASP:HB2	1:D:-5:GLN:HB2	1.96	0.47
1:A:-178:LEU:HD23	1:A:-13:VAL:HG13	1.97	0.47
1:C:40:CYS:HB3	1:C:89:TRP:NE1	2.30	0.47
1:A:-272:ARG:HD3	1:A:-269:GLY:HA2	1.97	0.46
1:C:-35:GLN:NE2	1:C:-35:GLN:H	2.13	0.46
1:D:-310:ILE:HG12	1:D:-309:PHE:N	2.30	0.46
1:D:5:LEU:O	1:D:9:LEU:HG	2.15	0.46
1:B:-192:ILE:HD12	1:C:38:SER:CB	2.46	0.46
1:B:-241:TRP:HA	1:B:-238:ILE:HD12	1.97	0.46
1:A:32:ASP:C	1:A:34:GLU:N	2.69	0.46
1:B:32:ASP:C	1:B:34:GLU:N	2.68	0.46
1:D:102:LEU:O	1:D:103:ASP:HB3	2.15	0.46
1:C:-155:ALA:O	1:C:-151:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-323:PHE:CG	1:A:-310:ILE:HD12	2.51	0.46
1:B:37:TYR:OH	1:C:-189:VAL:CG1	2.63	0.46
1:D:-216:PRO:HG2	1:D:-30:TRP:CE3	2.51	0.46
1:D:-325:GLU:O	1:D:-322:PRO:HD2	2.16	0.46
1:D:-358:ASN:ND2	1:D:-356:ASP:OD1	2.46	0.46
1:D:-5:GLN:HA	1:D:-5:GLN:OE1	2.16	0.46
1:D:-359:ILE:HG13	1:D:-309:PHE:HB3	1.96	0.45
1:A:81:ARG:CZ	1:A:93:ILE:HD11	2.47	0.45
1:C:-241:TRP:HA	1:C:-238:ILE:HD12	1.99	0.45
1:A:-248:LEU:HD13	1:A:-245:PRO:HA	1.98	0.45
1:B:41:ASN:HA	1:B:53:ARG:HG3	1.99	0.45
1:D:-308:TRP:HB3	1:D:-303:PHE:HE1	1.81	0.44
1:A:-155:ALA:O	1:A:-151:LYS:HG3	2.17	0.44
1:A:-310:ILE:HG12	1:A:-309:PHE:N	2.32	0.44
1:B:37:TYR:CZ	1:C:-189:VAL:C	2.86	0.44
1:C:-199:TYR:O	1:C:-198:GLU:HG3	2.17	0.44
1:C:-358:ASN:ND2	1:C:-356:ASP:OD1	2.50	0.44
1:B:-155:ALA:O	1:B:-151:LYS:HG3	2.17	0.44
1:C:66:GLU:HG3	1:C:75:THR:HG21	1.99	0.44
1:A:-248:LEU:HD21	1:A:-235:LEU:HD11	1.99	0.44
1:D:66:GLU:HG3	1:D:75:THR:HG21	1.99	0.44
1:B:-328:LYS:HZ2	2:H:37:ILE:HD11	1.80	0.44
1:B:77:ARG:HD3	1:B:97:GLN:O	2.18	0.44
1:B:-189:VAL:HG21	1:C:37:TYR:CD1	2.53	0.44
1:A:65:PRO:O	1:A:73:TYR:HB2	2.17	0.43
1:B:37:TYR:CZ	1:C:-5:GLN:OE1	2.71	0.43
1:A:81:ARG:HD3	1:A:89:TRP:CE3	2.52	0.43
1:A:-192:ILE:HD12	1:D:38:SER:HB2	1.99	0.43
1:B:-310:ILE:HG12	1:B:-309:PHE:N	2.33	0.43
1:B:21:GLU:HG2	1:B:53:ARG:HE	1.83	0.43
1:A:-358:ASN:ND2	1:A:-356:ASP:OD1	2.51	0.43
1:D:-206:ASP:O	1:D:-183:GLY:HA3	2.18	0.43
1:B:61:GLU:HG2	1:B:80:TYR:CE2	2.53	0.43
1:A:-241:TRP:HA	1:A:-238:ILE:HD12	2.01	0.43
1:A:-281:LEU:HA	1:A:-67:ALA:O	2.19	0.43
1:B:37:TYR:OH	1:C:-189:VAL:HB	2.19	0.42
1:D:-199:TYR:O	1:D:-198:GLU:HG3	2.19	0.42
1:A:-308:TRP:CD1	1:A:-307:ALA:N	2.87	0.42
1:A:96:SER:OG	1:A:97:GLN:NE2	2.49	0.42
1:D:-272:ARG:HD3	1:D:-269:GLY:HA2	2.01	0.42
1:A:40:CYS:HB3	1:A:89:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-199:TYR:OH	1:C:-196:GLY:HA2	2.20	0.42
1:C:43:THR:CG2	1:C:44:LEU:N	2.82	0.42
1:D:-368:ILE:HD13	1:D:-100:SER:HA	2.02	0.42
1:C:-147:ALA:N	4:C:130:HOH:O	2.53	0.42
1:B:31:LEU:HD13	4:B:135:HOH:O	2.19	0.41
1:A:-356:ASP:N	1:A:-356:ASP:OD1	2.44	0.41
1:D:-358:ASN:HB3	1:D:-356:ASP:OD1	2.21	0.41
1:B:-253:TYR:CE2	1:B:-245:PRO:HD3	2.55	0.41
1:B:-323:PHE:CG	1:B:-310:ILE:HD12	2.56	0.41
1:C:-308:TRP:HB3	1:C:-303:PHE:HE1	1.85	0.41
1:B:-360:TRP:HE3	1:B:-327:LEU:CD1	2.33	0.41
1:C:-303:PHE:HB3	1:C:-266:ILE:HD13	2.03	0.41
1:A:-212:TRP:N	1:A:-211:PRO:CD	2.83	0.41
1:A:-8:LYS:O	1:A:-5:GLN:HB3	2.21	0.41
1:B:-291:ILE:O	1:B:-291:ILE:HG13	2.20	0.41
1:B:81:ARG:CZ	1:B:93:ILE:HD11	2.51	0.41
1:B:-240:GLU:O	1:B:-237:PRO:HD2	2.21	0.40
1:C:-246:ASN:HA	1:C:-245:PRO:HD2	1.92	0.40
1:A:-291:ILE:HG13	1:A:-291:ILE:O	2.22	0.40
1:D:-287:LYS:HA	1:D:-287:LYS:HD3	1.90	0.40
1:B:-308:TRP:CD1	1:B:-307:ALA:N	2.90	0.40
1:C:-359:ILE:HG13	1:C:-309:PHE:CB	2.52	0.40
1:C:65:PRO:O	1:C:73:TYR:HB2	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	471/482 (98%)	455 (97%)	13 (3%)	3 (1%)	28 59
1	B	469/482 (97%)	452 (96%)	14 (3%)	3 (1%)	28 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	463/482 (96%)	448 (97%)	13 (3%)	2 (0%)	38	69
1	D	464/482 (96%)	444 (96%)	18 (4%)	2 (0%)	38	69
2	E	15/17 (88%)	15 (100%)	0	0	100	100
2	F	15/17 (88%)	15 (100%)	0	0	100	100
2	G	13/17 (76%)	13 (100%)	0	0	100	100
2	H	9/17 (53%)	9 (100%)	0	0	100	100
All	All	1919/1996 (96%)	1851 (96%)	58 (3%)	10 (0%)	32	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-202	ALA
1	B	-202	ALA
1	B	36	PRO
1	C	25	ASP
1	D	25	ASP
1	A	36	PRO
1	B	33	PRO
1	C	-202	ALA
1	D	-202	ALA
1	A	33	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/388 (98%)	360 (95%)	20 (5%)	26	56
1	B	378/388 (97%)	361 (96%)	17 (4%)	32	63
1	C	375/388 (97%)	356 (95%)	19 (5%)	28	58
1	D	376/388 (97%)	356 (95%)	20 (5%)	26	56
2	E	15/15 (100%)	14 (93%)	1 (7%)	19	44
2	F	15/15 (100%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	13/15 (87%)	11 (85%)	2 (15%)	3	8
2	H	10/15 (67%)	10 (100%)	0	100	100
All	All	1562/1612 (97%)	1483 (95%)	79 (5%)	28	58

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-369	LYS
1	A	-345	LYS
1	A	-341	LYS
1	A	-287	LYS
1	A	-213	THR
1	A	-197	ASN
1	A	-187	VAL
1	A	-112	PHE
1	A	-35	GLN
1	A	-33	SER
1	A	16	LEU
1	A	21	GLU
1	A	23	LEU
1	A	25	ASP
1	A	37	TYR
1	A	38	SER
1	A	46	GLN
1	A	99	GLU
1	A	102	LEU
1	A	103	ASP
1	B	-369	LYS
1	B	-345	LYS
1	B	-341	LYS
1	B	-310	ILE
1	B	-287	LYS
1	B	-233	LYS
1	B	-232	GLU
1	B	-197	ASN
1	B	-112	PHE
1	B	-33	SER
1	B	16	LEU
1	B	21	GLU
1	B	23	LEU
1	B	25	ASP

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Mol	Chain	Res	Type
1	B	31	LEU
1	B	37	TYR
1	B	99	GLU
1	C	-369	LYS
1	C	-345	LYS
1	C	-341	LYS
1	C	-310	ILE
1	C	-237	PRO
1	C	-233	LYS
1	C	-213	THR
1	C	-197	ASN
1	C	-112	PHE
1	C	-35	GLN
1	C	-33	SER
1	C	16	LEU
1	C	21	GLU
1	C	25	ASP
1	C	43	THR
1	C	46	GLN
1	C	59	LEU
1	C	92	LYS
1	C	99	GLU
1	D	-369	LYS
1	D	-345	LYS
1	D	-341	LYS
1	D	-310	ILE
1	D	-233	LYS
1	D	-225	SER
1	D	-213	THR
1	D	-197	ASN
1	D	-112	PHE
1	D	-35	GLN
1	D	-33	SER
1	D	5	LEU
1	D	16	LEU
1	D	21	GLU
1	D	25	ASP
1	D	43	THR
1	D	46	GLN
1	D	92	LYS
1	D	99	GLU
1	D	102	LEU

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Mol	Chain	Res	Type
2	E	27	GLN
2	G	28	ARG
2	G	29	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-352	ASN
1	A	-321	GLN
1	A	-169	ASN
1	A	-152	ASN
1	A	-35	GLN
1	B	-352	ASN
1	B	-321	GLN
1	B	-169	ASN
1	B	-152	ASN
1	B	-35	GLN
1	C	-352	ASN
1	C	-169	ASN
1	C	-152	ASN
1	C	-35	GLN
1	C	-3	ASN
1	D	-352	ASN
1	D	-169	ASN
1	D	-152	ASN
1	D	-35	GLN
1	D	-3	ASN
2	H	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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$
3	MAL	A	111	-	24,24,24	0.87	0	35,35,35	0.93	0
3	MAL	B	111	-	24,24,24	0.69	0	35,35,35	1.01	2 (5%)
3	MAL	C	111	-	24,24,24	0.61	0	35,35,35	1.14	2 (5%)
3	MAL	D	111	-	24,24,24	0.62	0	35,35,35	1.33	4 (11%)

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
3	MAL	A	111	-	-	0/8/48/48	0/2/2/2
3	MAL	B	111	-	-	0/8/48/48	0/2/2/2
3	MAL	C	111	-	-	0/8/48/48	0/2/2/2
3	MAL	D	111	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	111	MAL	O2'-C2'-C1'	-2.37	104.82	109.75
3	B	111	MAL	O6'-C6'-C5'	-2.22	103.86	111.34
3	B	111	MAL	O3-C3-C2	-2.22	105.53	110.36
3	D	111	MAL	C1'-C2'-C3'	2.18	114.60	110.65
3	C	111	MAL	C2'-C3'-C4'	2.55	114.90	109.61
3	C	111	MAL	C1'-C2'-C3'	2.62	115.38	110.65
3	D	111	MAL	O5-C5-C6	3.08	113.79	106.41
3	D	111	MAL	C1'-O5'-C5'	3.15	119.08	113.39

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	473/482 (98%)	0.26	7 (1%) 74 71	42, 54, 74, 113	0
1	B	471/482 (97%)	0.29	7 (1%) 74 71	43, 55, 69, 102	0
1	C	467/482 (96%)	0.44	28 (5%) 23 18	46, 61, 96, 111	0
1	D	468/482 (97%)	0.46	25 (5%) 27 21	46, 61, 97, 113	0
2	E	16/17 (94%)	0.67	2 (12%) 4 3	78, 93, 112, 125	0
2	F	16/17 (94%)	0.85	1 (6%) 21 16	82, 92, 113, 114	0
2	G	14/17 (82%)	2.46	10 (71%) 0 0	114, 116, 122, 127	0
2	H	10/17 (58%)	2.62	6 (60%) 0 0	115, 119, 134, 136	0
All	All	1935/1996 (96%)	0.40	86 (4%) 35 29	42, 58, 96, 136	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	PRO	7.2
1	D	27	TRP	5.6
1	C	27	TRP	5.1
1	D	-365	GLY	4.6
2	G	31	ALA	4.6
2	G	37	ILE	4.5
1	D	-86	LEU	4.5
1	B	37	TYR	4.3
1	A	37	TYR	4.2
2	H	37	ILE	4.2
1	C	-338	GLY	4.0
1	A	35	GLY	3.9
1	C	-367	GLU	3.9
1	D	-95	LEU	3.7
2	H	35	ARG	3.5
1	C	-197	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	32	ASP	3.4
2	H	39	ASP	3.4
2	G	41	VAL	3.3
2	G	38	PHE	3.2
1	C	-92	GLU	3.1
1	D	-337	ILE	3.1
1	D	-366	GLU	3.1
1	C	-268	LYS	3.0
1	A	103	ASP	3.0
1	D	-92	GLU	3.0
1	C	-266	ILE	2.9
1	C	-104	ILE	2.9
2	E	28	ARG	2.9
1	D	-278	PHE	2.9
2	H	41	VAL	2.9
1	D	-94	ALA	2.9
1	D	-266	ILE	2.9
1	C	-86	LEU	2.9
1	B	85	GLU	2.8
2	G	33	GLN	2.7
1	C	-286	ALA	2.7
2	G	39	ASP	2.7
2	H	40	SER	2.7
1	C	-81	GLY	2.6
1	C	-198	GLU	2.6
2	H	38	PHE	2.6
1	C	-91	PHE	2.6
1	D	-286	ALA	2.6
1	D	-334	THR	2.6
2	G	32	GLU	2.6
2	G	40	SER	2.6
1	C	-63	TYR	2.6
1	C	36	PRO	2.5
1	D	-262	ILE	2.5
1	D	-91	PHE	2.5
1	C	-300	TYR	2.5
1	C	-262	ILE	2.5
1	A	6	LEU	2.5
1	D	37	TYR	2.5
1	C	-100	SER	2.5
1	C	-317	THR	2.4
1	D	-81	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	27	GLN	2.4
1	B	6	LEU	2.4
1	D	-369	LYS	2.4
1	C	29	PRO	2.3
1	B	21	GLU	2.3
1	C	30	PRO	2.3
1	D	-321	GLN	2.3
1	C	-321	GLN	2.3
1	D	102	LEU	2.3
2	F	30	ARG	2.3
1	A	32	ASP	2.2
1	A	85	GLU	2.2
2	G	36	ILE	2.2
1	D	-265	ALA	2.2
1	D	103	ASP	2.2
1	D	-317	THR	2.2
1	A	67	TYR	2.2
1	C	-5	GLN	2.1
1	B	-68	VAL	2.1
1	C	-87	TYR	2.1
2	G	29	GLU	2.1
1	B	35	GLY	2.1
1	D	-59	LEU	2.1
1	C	-264	TYR	2.1
1	D	-363	LEU	2.0
1	C	-267	LEU	2.0
1	C	-90	LEU	2.0
1	C	-368	ILE	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(Å ²)	Q<0.9
3	MAL	B	111	23/23	0.94	0.17	-0.45	41,48,53,56	0
3	MAL	A	111	23/23	0.96	0.17	-0.74	39,47,52,53	0
3	MAL	D	111	23/23	0.95	0.15	-1.48	49,54,57,58	0
3	MAL	C	111	23/23	0.94	0.13	-1.56	48,54,59,59	0

6.5 Other polymers

There are no such residues in this entry.