Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 PM GMT

PDB ID	:	4P7H
Title	:	Structure of Human beta-Cardiac Myosin Motor Domain::GFP chimera
Authors	:	Winkelmann, D.A.; Miller, M.T.; Stock, A.M.
Deposited on	:	2014-03-27
Resolution	:	3.20 Å(reported)

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

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

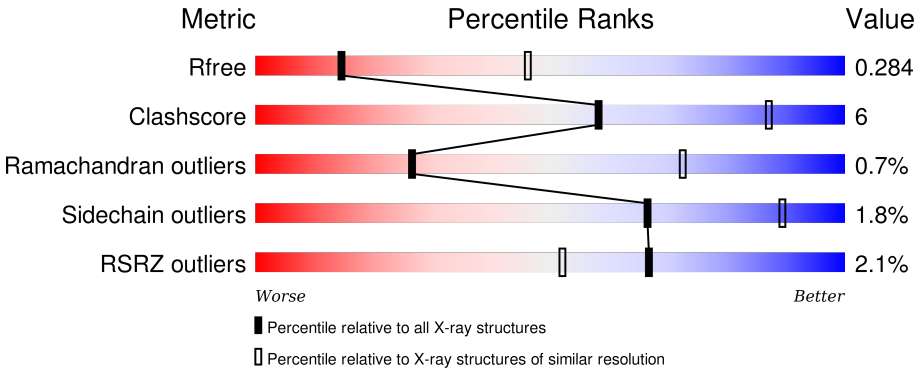
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	1023	% 78% 16% • 5%
1	B	1023	3% 75% 17% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15459 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 Myosin-7,Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	972	Total	C	N	O	S	0	0	0
			7798	4977	1326	1457	38			
1	B	953	Total	C	N	O	S	0	0	0
			7646	4881	1296	1431	38			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	THR	-	linker	UNP P12883
A	789	GLN	-	linker	UNP P12883
A	790	ALA	-	linker	UNP P12883
A	791	ALA	-	linker	UNP P12883
A	853	CRO	SER	chromophore	UNP P42212
A	853	CRO	TYR	chromophore	UNP P42212
A	853	CRO	GLY	chromophore	UNP P42212
A	867	ARG	GLN	engineered mutation	UNP P42212
A	888	ASN	LYS	engineered mutation	UNP P42212
A	950	ALA	VAL	engineered mutation	UNP P42212
A	954	THR	ILE	engineered mutation	UNP P42212
A	962	GLY	SER	engineered mutation	UNP P42212
A	977	ASN	ASP	engineered mutation	UNP P42212
B	788	THR	-	linker	UNP P12883
B	789	GLN	-	linker	UNP P12883
B	790	ALA	-	linker	UNP P12883
B	791	ALA	-	linker	UNP P12883
B	853	CRO	SER	chromophore	UNP P42212
B	853	CRO	TYR	chromophore	UNP P42212
B	853	CRO	GLY	chromophore	UNP P42212
B	867	ARG	GLN	engineered mutation	UNP P42212
B	888	ASN	LYS	engineered mutation	UNP P42212
B	950	ALA	VAL	engineered mutation	UNP P42212
B	954	THR	ILE	engineered mutation	UNP P42212
B	962	GLY	SER	engineered mutation	UNP P42212

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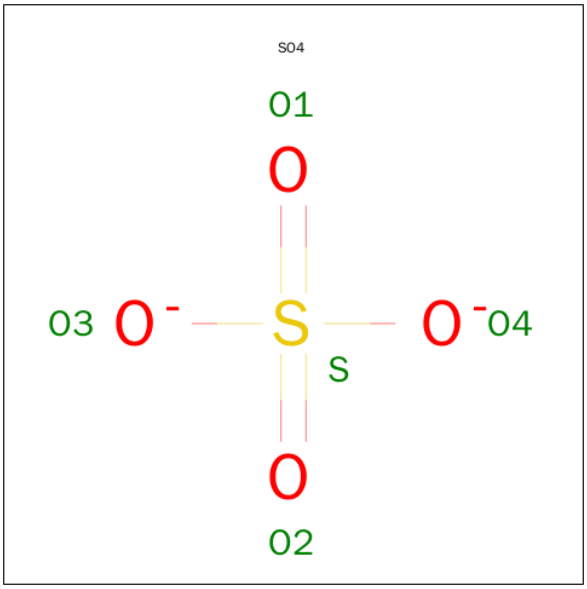
Chain	Residue	Modelled	Actual	Comment	Reference
B	977	ASN	ASP	engineered mutation	UNP P42212

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

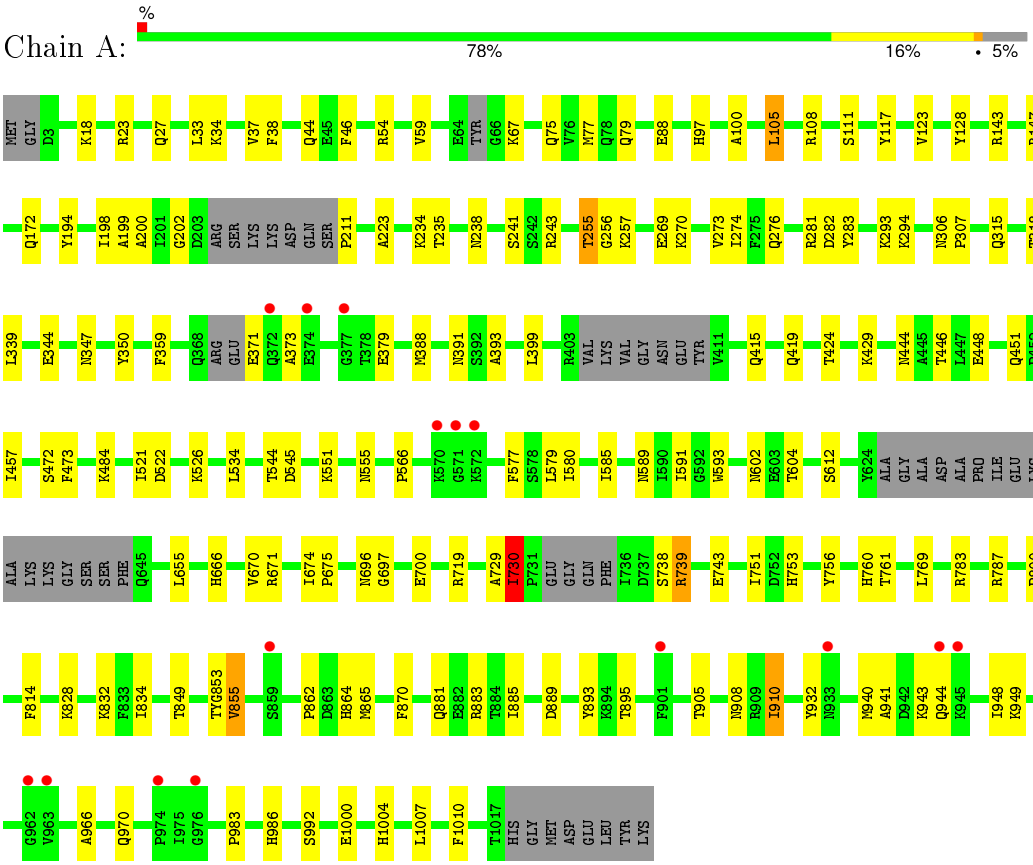
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	3	Total O 3 3	0	0

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.

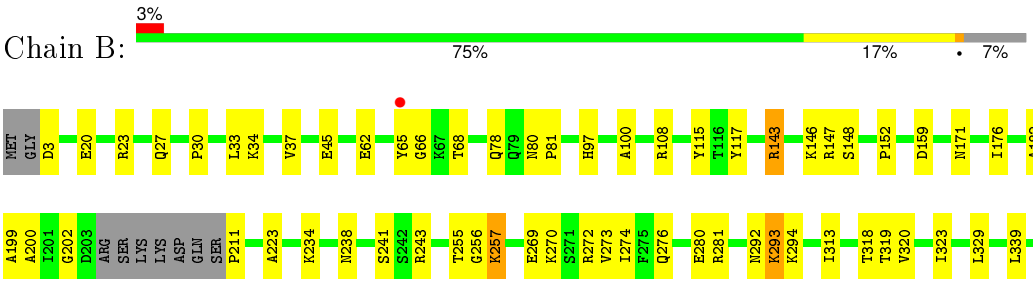
- Molecule 1: Myosin-7,Green fluorescent protein

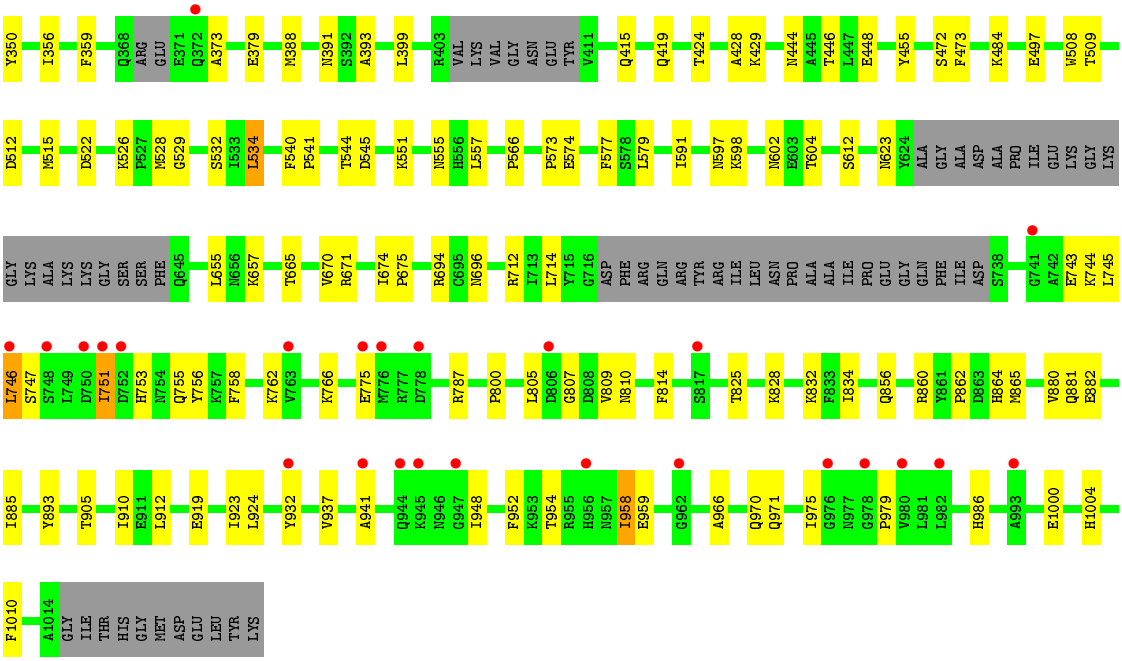
Chain A:



- Molecule 1: Myosin-7,Green fluorescent protein

Chain B:




Y350 I356 F359 Q368 ARG GLU E371 Q372 A373 E379 M388 N391 S392 A393 L399 R403 VAL LYS VAL GLY ASN GLU TYR V411 Q415 Q419 T424 A428 K429 N444 A445 T446 L447 E448 Y455 S472 F473 K484 E497 W508 T509
D512 M515 D522 K526 P527 M528 G529 S532 I533 L534 P540 P541 T544 D545 K551 N555 H556 L557 P566 P573 E574 F577 S578 L579 I591 N597 K598 N602 E603 T604 S612 N623 Y624 ALA GLY ALA ASP ALA PRO ILE GLU LYS GLY LYS
GLY LYS ALA LYS LYS GLY SER SER PHE Q645 L655 N656 K657 T665 V670 R671 I674 P675 R694 C695 M696 R712 I713 L714 Y715 G716 ASP PHE ARG GLN ARG TYR ARG ILE LEU ASN PRO ALA ALA ILE PRO GLU GLY GLN PHE ILE ASP S738 G741 A742 E743 K744 L745
L746 S747 S748 L749 D750 I751 D752 H753 N754 Q755 Y756 K757 F758 K762 V763 K766 E775 M776 R777 D778 R787 P800 L805 D806 G807 D808 V809 N810 F814 S817 T825 K828 K832 F833 I834 Q856 R860 Y861 P862 D863 H864 M865 V880 Q881 E882
I885 Y893 T905 I910 E911 L912 E919 I923 L924 Y932 V937 A941 Q944 K945 N946 G947 I948 F952 K953 T954 R955 H956 N957 I958 E959 G962 A966 Q970 Q971 I975 G976 N977 G978 P979 V980 L981 L982 H986 A993 E1000 H1004
F1010 A1014 GLY ILE THR HIS GLY MET ASP GLU LEU TYR LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.69Å 97.73Å 118.61Å 71.06° 82.67° 75.08°	Depositor
Resolution (Å)	37.94 – 3.20 55.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (37.94-3.20) 76.3 (55.79-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.226 , 0.284 0.233 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (6.30%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 36508 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	15459	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CRO

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	0.21	0/7941	0.36	0/10709
1	B	0.21	0/7787	0.36	0/10501
All	All	0.21	0/15728	0.36	0/21210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7798	0	7717	88	0
1	B	7646	0	7558	93	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
All	All	15459	0	15275	181	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 (181) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ALA:HB1	1:A:200:ALA:HA	1.63	0.79
1:B:199:ALA:HB1	1:B:200:ALA:HA	1.65	0.77
1:B:671:ARG:HD2	1:B:696:ASN:HB2	1.68	0.76
1:A:143:ARG:NH1	1:A:159:ASP:OD2	2.22	0.73
1:A:211:PRO:HG2	1:A:446:THR:HG22	1.76	0.67
1:A:751:ILE:HD11	1:A:769:LEU:HD11	1.76	0.67
1:B:787:ARG:HE	1:B:979:PRO:HB2	1.61	0.66
1:B:273:VAL:HG13	1:B:274:ILE:HG23	1.78	0.65
1:A:783:ARG:HG2	1:A:787:ARG:HH12	1.63	0.64
1:A:293:LYS:HB3	1:A:329:LEU:HD23	1.81	0.63
1:B:856:GLN:HE22	1:B:970:GLN:HE22	1.46	0.61
1:B:318:THR:HG23	1:B:319:THR:HG23	1.84	0.60
1:B:551:LYS:O	1:B:555:ASN:ND2	2.29	0.59
1:A:234:LYS:HB3	1:A:281:ARG:HG2	1.84	0.59
1:B:747:SER:HA	1:B:753:HIS:HE1	1.67	0.59
1:B:143:ARG:NH1	1:B:159:ASP:OD2	2.36	0.58
1:A:719:ARG:HH21	1:A:738:SER:HB3	1.69	0.58
1:B:941:ALA:HB2	1:B:948:ILE:HG22	1.85	0.58
1:B:255:THR:N	1:B:256:GLY:HA2	2.18	0.58
1:A:238:ASN:HB3	1:A:241:SER:HB2	1.86	0.57
1:A:223:ALA:HA	1:A:339:LEU:HD11	1.86	0.57
1:A:318:THR:HG23	1:A:319:THR:HG23	1.87	0.57
1:A:273:VAL:HG13	1:A:274:ILE:HG23	1.85	0.57
1:A:347:ASN:HA	1:A:350:TYR:HD2	1.69	0.56
1:B:347:ASN:HA	1:B:350:TYR:HD2	1.70	0.56
1:A:484:LYS:HD2	1:A:521:ILE:HD13	1.88	0.56
1:B:825:THR:O	1:B:860:ARG:NH1	2.39	0.55
1:B:602:ASN:OD1	1:B:604:THR:OG1	2.24	0.55
1:A:255:THR:N	1:A:256:GLY:HA2	2.21	0.55
1:B:3:ASP:HB3	1:B:20:GLU:HG3	1.88	0.55
1:B:146:LYS:O	1:B:148:SER:N	2.38	0.55
1:A:143:ARG:HA	1:A:143:ARG:HH11	1.71	0.54
1:B:202:GLY:HA2	1:B:257:LYS:HD2	1.89	0.54
1:B:37:VAL:HG12	1:B:78:GLN:HA	1.90	0.54
1:B:194:TYR:O	1:B:198:ILE:HG12	2.07	0.54
1:A:881:GLN:NE2	1:A:970:GLN:OE1	2.40	0.54
1:A:954:THR:HB	1:A:966:ALA:HB3	1.90	0.54
1:A:202:GLY:HA2	1:A:257:LYS:HD2	1.89	0.54
1:B:881:GLN:OE1	1:B:970:GLN:NE2	2.42	0.53
1:A:883:ARG:HB2	1:A:895:THR:HB	1.90	0.53
1:B:292:ASN:O	1:B:294:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASP:N	1:B:20:GLU:OE1	2.41	0.53
1:B:828:LYS:HG3	1:B:1010:PHE:HE1	1.74	0.53
1:A:828:LYS:HG3	1:A:1010:PHE:HE1	1.75	0.52
1:A:117:TYR:HB3	1:A:147:ARG:HH21	1.74	0.52
1:B:954:THR:HB	1:B:966:ALA:HB3	1.91	0.52
1:B:270:LYS:HB3	1:B:429:LYS:HB3	1.91	0.52
1:A:194:TYR:O	1:A:198:ILE:HG12	2.09	0.51
1:B:753:HIS:O	1:B:755:GLN:N	2.37	0.51
1:B:33:LEU:HD22	1:B:775:GLU:HG2	1.91	0.51
1:A:739:ARG:NH1	1:A:743:GLU:OE2	2.44	0.51
1:B:714:LEU:HD23	1:B:762:LYS:HG3	1.92	0.51
1:A:415:GLN:HB3	1:A:419:GLN:HB2	1.93	0.51
1:A:849:THR:OG1	1:A:932:TYR:OH	2.27	0.51
1:B:753:HIS:HA	1:B:756:TYR:HE2	1.76	0.51
1:A:941:ALA:HB2	1:A:948:ILE:HG22	1.93	0.50
1:B:958:ILE:HG22	1:B:959:GLU:H	1.75	0.50
1:A:855:VAL:HG13	1:A:908:ASN:HD22	1.76	0.50
1:A:671:ARG:HD2	1:A:696:ASN:HB2	1.93	0.50
1:A:589:ASN:O	1:A:593:TRP:NE1	2.45	0.50
1:B:344:GLU:OE1	1:B:344:GLU:N	2.43	0.50
1:B:320:VAL:HB	1:B:323:ILE:HB	1.93	0.50
1:A:54:ARG:HG3	1:A:59:VAL:HG22	1.92	0.50
1:A:448:GLU:OE1	1:A:453:ARG:NH2	2.42	0.50
1:A:172:GLN:HB2	1:A:457:ILE:HG12	1.92	0.50
1:B:391:ASN:O	1:B:393:ALA:N	2.43	0.50
1:B:832:LYS:HE2	1:B:834:ILE:HD11	1.93	0.50
1:A:128:TYR:HE2	1:A:675:PRO:HD2	1.77	0.49
1:B:937:VAL:HG12	1:B:952:PHE:CG	2.47	0.49
1:B:223:ALA:HA	1:B:339:LEU:HD11	1.93	0.49
1:A:544:THR:OG1	1:A:545:ASP:N	2.45	0.49
1:A:444:ASN:O	1:A:448:GLU:HG2	2.12	0.49
1:A:23:ARG:O	1:A:27:GLN:HG2	2.12	0.49
1:A:832:LYS:HE2	1:A:834:ILE:HD11	1.93	0.49
1:A:344:GLU:N	1:A:344:GLU:OE1	2.46	0.49
1:B:923:ILE:HG22	1:B:924:LEU:HG	1.95	0.48
1:A:870:PHE:HB2	1:A:983:PRO:HD3	1.96	0.48
1:B:809:VAL:HG12	1:B:814:PHE:HE2	1.78	0.48
1:A:105:LEU:HD21	1:A:123:VAL:HG11	1.95	0.48
1:B:176:ILE:HG12	1:B:670:VAL:HB	1.96	0.48
1:B:97:HIS:CE1	1:B:100:ALA:HB2	2.49	0.48
1:B:444:ASN:O	1:B:448:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:LYS:HA	1:B:747:SER:HB3	1.95	0.47
1:B:885:ILE:HB	1:B:893:TYR:HB2	1.95	0.47
1:A:809:VAL:HG12	1:A:814:PHE:HE2	1.79	0.47
1:B:182:ALA:HA	1:B:674:ILE:HB	1.95	0.47
1:A:940:MET:O	1:A:949:LYS:N	2.43	0.47
1:B:746:LEU:HD23	1:B:751:ILE:HD11	1.96	0.47
1:A:602:ASN:OD1	1:A:604:THR:OG1	2.27	0.47
1:B:885:ILE:HD12	1:B:893:TYR:HD2	1.79	0.47
1:B:472:SER:OG	1:B:473:PHE:N	2.46	0.46
1:B:522:ASP:O	1:B:526:LYS:HB2	2.16	0.46
1:B:415:GLN:HB3	1:B:419:GLN:HB2	1.96	0.46
1:A:551:LYS:O	1:A:555:ASN:ND2	2.33	0.46
1:A:862:PRO:HG2	1:A:865:MET:HB2	1.97	0.46
1:A:864:HIS:CD2	1:A:865:MET:HG3	2.50	0.46
1:B:62:GLU:HB3	1:B:68:THR:HG22	1.98	0.46
1:B:23:ARG:O	1:B:27:GLN:HG2	2.16	0.46
1:B:862:PRO:HG2	1:B:865:MET:HB2	1.97	0.46
1:B:512:ASP:HB3	1:B:515:MET:HG2	1.98	0.46
1:B:399:LEU:HD11	1:B:424:THR:HG22	1.97	0.46
1:A:674:ILE:HA	1:A:675:PRO:HD3	1.84	0.45
1:B:882:GLU:HB2	1:B:971:GLN:HB2	1.98	0.45
1:B:864:HIS:CD2	1:B:865:MET:HG3	2.51	0.45
1:B:529:GLY:H	1:B:532:SER:HB3	1.81	0.45
1:A:270:LYS:HB3	1:A:429:LYS:HB3	1.99	0.45
1:A:800:PRO:HB2	1:A:905:THR:HG22	1.98	0.45
1:A:760:HIS:HA	1:A:761:THR:HA	1.48	0.45
1:A:697:GLY:HA2	1:A:700:GLU:HB3	1.98	0.45
1:B:484:LYS:HG3	1:B:655:LEU:HD21	1.97	0.45
1:B:108:ARG:NH1	1:B:115:TYR:O	2.50	0.45
1:B:234:LYS:HB3	1:B:281:ARG:HG2	1.98	0.45
1:A:67:LYS:H	1:A:67:LYS:HD2	1.81	0.45
1:A:566:PRO:HD3	1:A:577:PHE:HA	1.99	0.45
1:A:75:GLN:OE1	1:A:75:GLN:N	2.50	0.45
1:A:97:HIS:CE1	1:A:100:ALA:HB2	2.52	0.44
1:B:805:LEU:HD12	1:B:910:ILE:HD13	2.00	0.44
1:B:388:MET:O	1:B:612:SER:OG	2.32	0.44
1:B:276:GLN:HE22	1:B:313:ILE:HA	1.82	0.44
1:B:566:PRO:HD3	1:B:577:PHE:HA	1.98	0.44
1:A:388:MET:O	1:A:612:SER:OG	2.31	0.44
1:B:293:LYS:HB3	1:B:329:LEU:HD23	2.00	0.44
1:A:805:LEU:HD12	1:A:910:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ILE:O	1:B:199:ALA:HB3	2.18	0.44
1:B:45:GLU:OE2	1:B:694:ARG:NH2	2.47	0.44
1:B:238:ASN:HB3	1:B:241:SER:HB2	2.00	0.44
1:A:958:ILE:HG22	1:A:959:GLU:H	1.82	0.44
1:B:65:TYR:HB2	1:B:66:GLY:HA2	1.99	0.44
1:A:992:SER:HB3	1:A:1007:LEU:HD11	1.99	0.44
1:A:729:ALA:O	1:A:730:ILE:HG12	2.18	0.44
1:A:484:LYS:HG3	1:A:655:LEU:HD21	2.00	0.43
1:B:243:ARG:HB3	1:B:269:GLU:HG2	2.00	0.43
1:A:198:ILE:O	1:A:199:ALA:HB3	2.18	0.43
1:A:670:VAL:O	1:A:671:ARG:NH1	2.51	0.43
1:B:810:ASN:ND2	1:B:919:GLU:OE2	2.50	0.43
1:A:276:GLN:HG2	1:A:315:GLN:HB2	2.00	0.43
1:B:211:PRO:HG2	1:B:446:THR:HG22	1.99	0.43
1:A:33:LEU:O	1:A:34:LYS:HG2	2.18	0.43
1:A:391:ASN:C	1:A:393:ALA:H	2.22	0.43
1:B:171:ASN:HB3	1:B:665:THR:HG22	2.00	0.43
1:A:580:ILE:HG12	1:A:585:ILE:HG12	2.01	0.43
1:A:1000:GLU:HB3	1:A:1004:HIS:CE1	2.54	0.43
1:B:33:LEU:O	1:B:34:LYS:HG2	2.18	0.42
1:B:743:GLU:HA	1:B:758:PHE:CZ	2.53	0.42
1:A:169:ARG:HG2	1:A:455:TYR:OH	2.19	0.42
1:A:282:ASP:OD1	1:A:283:TYR:N	2.44	0.42
1:A:885:ILE:HB	1:A:893:TYR:HB2	2.00	0.42
1:A:18:LYS:HE3	1:A:111:SER:HB3	2.00	0.42
1:B:880:VAL:HG23	1:B:975:ILE:HG12	2.01	0.42
1:A:243:ARG:HB3	1:A:269:GLU:HG2	2.01	0.42
1:A:472:SER:OG	1:A:473:PHE:N	2.49	0.42
1:B:800:PRO:HB2	1:B:905:THR:HG22	2.00	0.42
1:A:38:PHE:HB2	1:A:77:MET:HB2	2.02	0.42
1:B:674:ILE:HA	1:B:675:PRO:HD3	1.84	0.42
1:A:88:GLU:HG2	1:A:108:ARG:HH21	1.85	0.41
1:B:497:GLU:OE2	1:B:712:ARG:NH2	2.53	0.41
1:A:753:HIS:HA	1:A:756:TYR:CE2	2.56	0.41
1:A:202:GLY:HA3	1:A:451:GLN:NE2	2.36	0.41
1:B:807:GLY:HA2	1:B:912:LEU:HB3	2.02	0.41
1:B:856:GLN:HE22	1:B:970:GLN:NE2	2.15	0.41
1:B:80:ASN:HA	1:B:81:PRO:HD3	1.93	0.41
1:A:853:CRO:O2	1:A:883:ARG:NH2	2.37	0.41
1:A:37:VAL:HA	1:A:79:GLN:HG3	2.02	0.41
1:B:755:GLN:HB3	1:B:766:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:HA	1:B:143:ARG:HH11	1.86	0.41
1:A:241:SER:OG	2:A:1101:SO4:O3	2.35	0.41
1:B:272:ARG:NH1	1:B:280:GLU:OE1	2.51	0.41
1:B:597:ASN:OD1	1:B:598:LYS:N	2.52	0.41
1:A:522:ASP:O	1:A:526:LYS:HB2	2.19	0.41
1:B:534:LEU:HD22	1:B:597:ASN:HD22	1.86	0.41
1:A:943:LYS:HA	1:A:944:GLN:HA	1.81	0.41
1:B:544:THR:OG1	1:B:545:ASP:N	2.54	0.40
1:B:540:PHE:HA	1:B:541:PRO:HD3	1.94	0.40
1:B:657:LYS:HE3	1:B:657:LYS:HB2	1.87	0.40
1:B:356:ILE:HG23	1:B:428:ALA:HB1	2.04	0.40
1:A:371:GLU:OE1	1:A:371:GLU:N	2.54	0.40
1:A:306:ASN:HA	1:A:307:PRO:HD3	1.88	0.40
1:B:1000:GLU:HB3	1:B:1004:HIS:CE1	2.57	0.40
1:A:44:GLN:C	1:A:46:PHE:H	2.25	0.40
1:B:117:TYR:CZ	1:B:152:PRO:HA	2.55	0.40
1:A:399:LEU:HD11	1:A:424:THR:HG22	2.04	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	955/1023 (93%)	901 (94%)	50 (5%)	4 (0%)	39	80
1	B	938/1023 (92%)	871 (93%)	57 (6%)	10 (1%)	17	62
All	All	1893/2046 (92%)	1772 (94%)	107 (6%)	14 (1%)	26	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	ARG

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Mol	Chain	Res	Type
1	B	379	GLU
1	A	379	GLU
1	B	293	LYS
1	B	373	ALA
1	B	591	ILE
1	A	373	ALA
1	B	147	ARG
1	B	623	ASN
1	A	730	ILE
1	B	30	PRO
1	B	751	ILE
1	A	591	ILE
1	B	573	PRO

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	842/881 (96%)	827 (98%)	15 (2%)	66	89
1	B	826/881 (94%)	811 (98%)	15 (2%)	66	89
All	All	1668/1762 (95%)	1638 (98%)	30 (2%)	66	89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	235	THR
1	A	255	THR
1	A	294	LYS
1	A	359	PHE
1	A	455	TYR
1	A	534	LEU
1	A	579	LEU
1	A	666	HIS
1	A	730	ILE

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Mol	Chain	Res	Type
1	A	739	ARG
1	A	855	VAL
1	A	889	ASP
1	A	910	ILE
1	A	986	HIS
1	B	257	LYS
1	B	359	PHE
1	B	455	TYR
1	B	508	TRP
1	B	509	THR
1	B	528	MET
1	B	534	LEU
1	B	557	LEU
1	B	574	GLU
1	B	579	LEU
1	B	745	LEU
1	B	746	LEU
1	B	932	TYR
1	B	958	ILE
1	B	986	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	881	GLN
1	B	964	GLN
1	B	970	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CRO	A	853	1	23,23,24	3.44	4 (17%)	29,32,34	2.13	5 (17%)
1	CRO	B	853	1	23,23,24	3.44	4 (17%)	29,32,34	2.15	5 (17%)

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
1	CRO	A	853	1	-	0/12/31/32	0/2/2/2
1	CRO	B	853	1	-	0/12/31/32	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	853	CRO	C2-N3	-2.69	1.34	1.39
1	A	853	CRO	C2-N3	-2.66	1.34	1.39
1	B	853	CRO	C1-N2	2.53	1.36	1.32
1	A	853	CRO	C1-N2	2.56	1.36	1.32
1	A	853	CRO	O2-C2	2.69	1.28	1.23
1	B	853	CRO	O2-C2	2.74	1.28	1.23
1	A	853	CRO	CB2-CA2	15.54	1.48	1.35
1	B	853	CRO	CB2-CA2	15.55	1.48	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	853	CRO	O2-C2-CA2	-6.89	127.23	130.95
1	A	853	CRO	O2-C2-CA2	-6.70	127.33	130.95
1	A	853	CRO	CG2-CB2-CA2	-6.57	121.68	130.22
1	B	853	CRO	CG2-CB2-CA2	-6.31	122.03	130.22
1	B	853	CRO	C2-CA2-N2	-2.58	106.85	108.91
1	A	853	CRO	C2-CA2-N2	-2.47	106.94	108.91
1	A	853	CRO	CA2-N2-C1	2.12	107.64	105.71
1	B	853	CRO	CA2-N2-C1	2.16	107.67	105.71
1	A	853	CRO	CA2-C2-N3	4.19	105.50	103.40
1	B	853	CRO	CA2-C2-N3	4.25	105.53	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	853	CRO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1101	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	B	1101	-	4,4,4	0.22	0	6,6,6	0.09	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	SO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1101	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	971/1023 (94%)	-0.04	15 (1%)	76	63	18, 61, 96, 130	0
1	B	952/1023 (93%)	-0.00	26 (2%)	58	44	18, 51, 111, 139	0
All	All	1923/2046 (93%)	-0.02	41 (2%)	67	52	18, 57, 105, 139	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	752	ASP	5.0
1	B	775	GLU	4.3
1	A	963	VAL	3.6
1	B	993	ALA	3.5
1	A	572	LYS	3.2
1	B	944	GLN	3.2
1	B	978	GLY	3.1
1	A	976	GLY	3.0
1	B	982	LEU	2.8
1	B	962	GLY	2.8
1	A	933	ASN	2.8
1	B	751	ILE	2.8
1	B	746	LEU	2.7
1	B	932	TYR	2.7
1	B	956	HIS	2.7
1	A	944	GLN	2.6
1	A	372	GLN	2.6
1	B	763	VAL	2.5
1	B	945	LYS	2.5
1	B	741	GLY	2.5
1	B	750	ASP	2.5
1	B	778	ASP	2.4
1	A	945	LYS	2.4
1	A	374	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	377	GLY	2.3
1	A	901	PHE	2.3
1	B	372	GLN	2.3
1	A	571	GLY	2.2
1	A	859	SER	2.2
1	B	776	MET	2.2
1	B	806	ASP	2.2
1	B	817	SER	2.2
1	B	980	VAL	2.1
1	A	974	PRO	2.0
1	B	65	TYR	2.0
1	B	748	SER	2.0
1	A	962	GLY	2.0
1	B	976	GLY	2.0
1	B	947	GLY	2.0
1	A	570	LYS	2.0
1	B	941	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CRO	A	853	22/23	0.91	0.25	-	58,66,79,85	0
1	CRO	B	853	22/23	0.93	0.23	-	58,70,75,76	0

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, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	1101	5/5	0.97	0.17	0.20	41,50,59,70	0
2	SO4	B	1101	5/5	0.96	0.14	-1.34	46,47,52,70	0

6.5 Other polymers (i)

There are no such residues in this entry.