Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:32 AM GMT

PDB ID	:	2R4F
Title	:	Substituted Pyrazoles as Hepatselective HMG-COA reductase inhibitors
Authors	:	Pavlovsky, A.; Pfefferkorn, J.A.; Harris, M.S.; Finzel, B.C.
Deposited on	:	2007-08-31
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

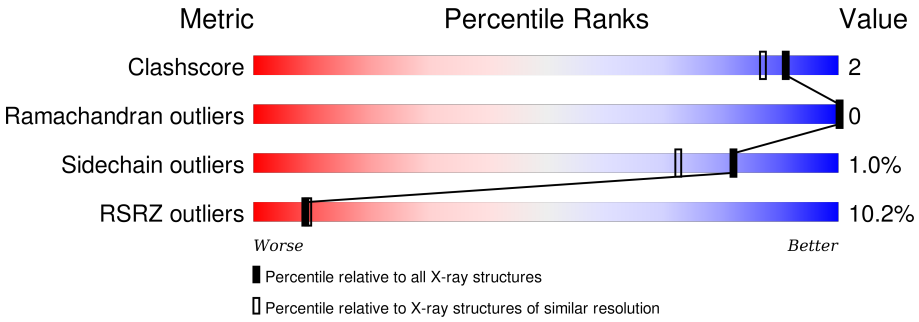
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	441	9% 89% 6% 5%
1	B	441	10% 88% • 8%
1	C	441	10% 88% • 8%
1	D	441	8% 85% • 11%

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	SO4	B	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13374 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3123	1945	548	600	30			
1	B	405	Total	C	N	O	S	0	2	0
			3013	1874	529	580	30			
1	C	404	Total	C	N	O	S	0	3	0
			2997	1862	524	579	32			
1	D	394	Total	C	N	O	S	0	3	0
			2921	1815	512	564	30			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	EXPRESSION TAG	UNP P04035
A	436	HIS	-	EXPRESSION TAG	UNP P04035
A	437	HIS	-	EXPRESSION TAG	UNP P04035
A	438	HIS	-	EXPRESSION TAG	UNP P04035
A	439	HIS	-	EXPRESSION TAG	UNP P04035
A	440	HIS	-	EXPRESSION TAG	UNP P04035
A	485	ILE	MET	ENGINEERED	UNP P04035
B	435	HIS	-	EXPRESSION TAG	UNP P04035
B	436	HIS	-	EXPRESSION TAG	UNP P04035
B	437	HIS	-	EXPRESSION TAG	UNP P04035
B	438	HIS	-	EXPRESSION TAG	UNP P04035
B	439	HIS	-	EXPRESSION TAG	UNP P04035
B	440	HIS	-	EXPRESSION TAG	UNP P04035
B	485	ILE	MET	ENGINEERED	UNP P04035
C	435	HIS	-	EXPRESSION TAG	UNP P04035
C	436	HIS	-	EXPRESSION TAG	UNP P04035
C	437	HIS	-	EXPRESSION TAG	UNP P04035
C	438	HIS	-	EXPRESSION TAG	UNP P04035
C	439	HIS	-	EXPRESSION TAG	UNP P04035
C	440	HIS	-	EXPRESSION TAG	UNP P04035
C	485	ILE	MET	ENGINEERED	UNP P04035

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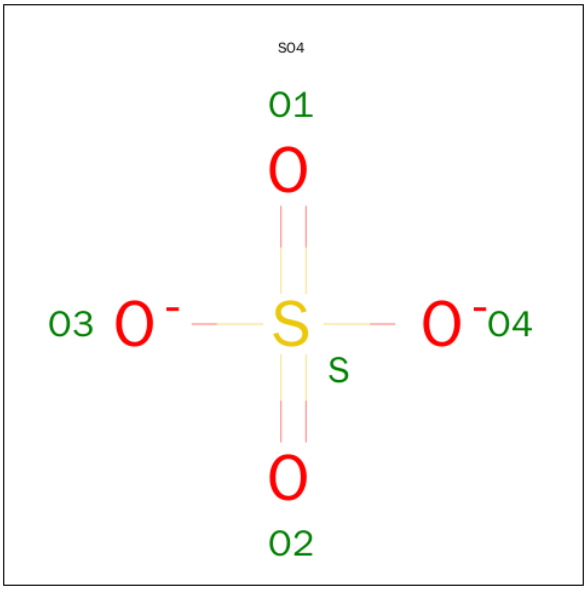
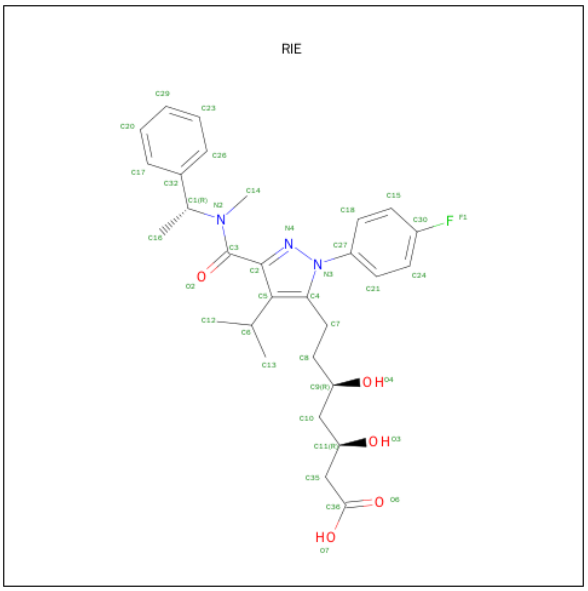
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	EXPRESSION TAG	UNP P04035
D	436	HIS	-	EXPRESSION TAG	UNP P04035
D	437	HIS	-	EXPRESSION TAG	UNP P04035
D	438	HIS	-	EXPRESSION TAG	UNP P04035
D	439	HIS	-	EXPRESSION TAG	UNP P04035
D	440	HIS	-	EXPRESSION TAG	UNP P04035
D	485	ILE	MET	ENGINEERED	UNP P04035

- 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
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is (3R,5R)-7-[1-(4-FLUOROPHENYL)-4-(1-METHYLETHYL)-3-{METHYL[(1R)-1-PHENYLETHYL]CARBAMOYL}-1H-PYRAZOL-5-YL]-3,5-DIHYDROXYHEPTANOIC ACID (three-letter code: RIE) (formula: $C_{29}H_{36}FN_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	29	1	3	5		
3	B	1	Total	C	F	N	O	0	0
			38	29	1	3	5		
3	C	1	Total	C	F	N	O	0	0
			38	29	1	3	5		
3	D	1	Total	C	F	N	O	0	0
			38	29	1	3	5		

- Molecule 4 is water.

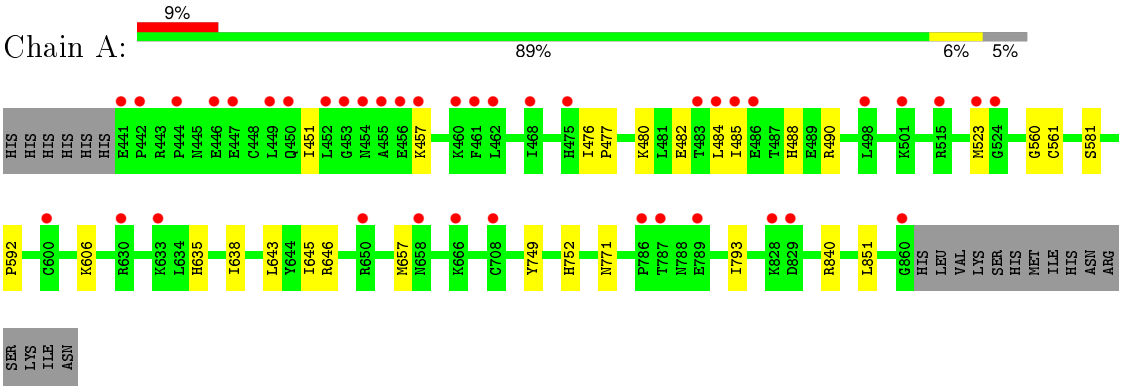
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total	O	0	0
			299	299		
4	B	291	Total	O	0	0
			291	291		
4	C	271	Total	O	0	0
			271	271		
4	D	287	Total	O	0	0
			287	287		

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.

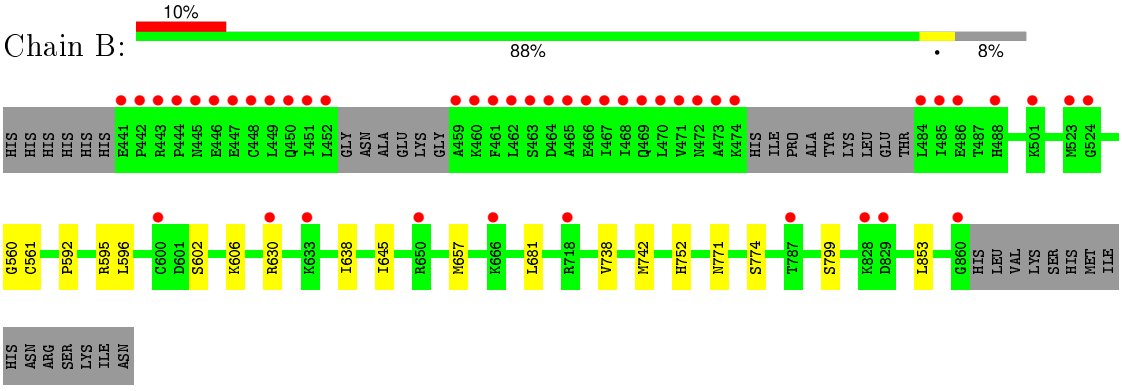
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain A:



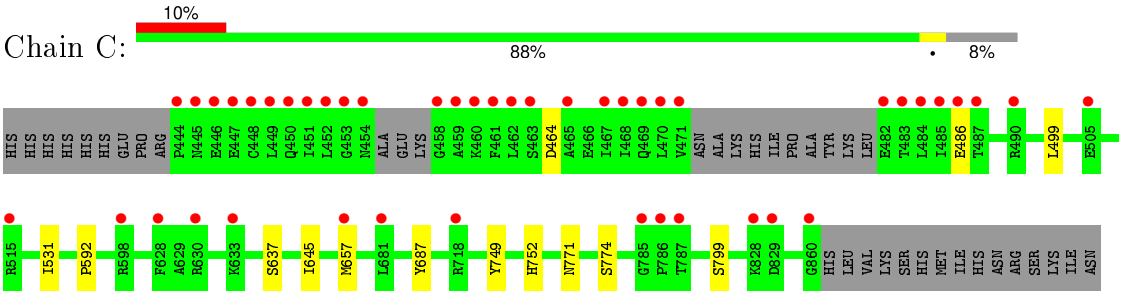
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain B:



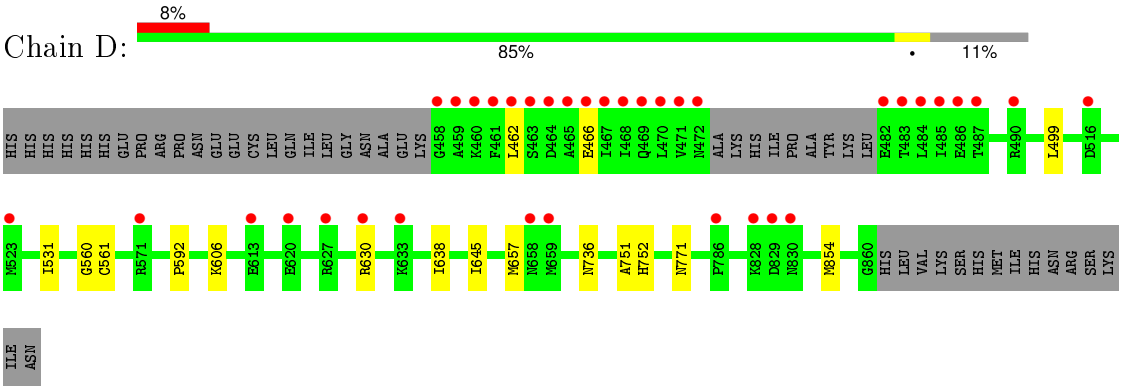
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain C:



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain D:


8%
85%
11%
HIS HIS HIS HIS HIS HIS GLU PRO ARG PRO ASN GLU GLU CYS LEU GLN ILE LEU GLY ASN ALA GLU LYS G458 A459 K460 F461 L462 S463 D464 A465 E466 T467 I468 Q469 L470 V471 N472 ALA LYS HIS ILE PRO ALA TYR LYS LEU E482 T483 L484 I485 E486 T487 N490 L499 D516
M523 I531 G560 C561 R571 P592 K606 E613 E620 R627 R630 K633 I638 I645 M657 N658 M659 N736 A751 H752 N771 P786 K828 D829 M830 M854 G860 HIS LEU VAL LYS SER HIS MET ILE HIS ASN ARG SER LYS
ILE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.62Å 135.33Å 82.84Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	39.54 – 1.70 39.54 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.7 (39.54-1.70) 89.0 (39.54-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.234 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.8	EDS
Estimated twinning fraction	0.144 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 186474 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13374	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: RIE, SO4

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	0.30	0/3168	0.45	0/4283
1	B	0.30	0/3063	0.44	0/4138
1	C	0.30	0/3051	0.44	0/4121
1	D	0.30	0/2975	0.45	0/4020
All	All	0.30	0/12257	0.45	0/16562

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	3123	0	3160	15	0
1	B	3013	0	3049	10	0
1	C	2997	0	3025	13	0
1	D	2921	0	2951	21	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	38	0	35	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	35	2	0
3	C	38	0	35	2	0
3	D	38	0	35	1	0
4	A	299	0	0	0	0
4	B	291	0	0	0	0
4	C	271	0	0	0	0
4	D	287	0	0	0	0
All	All	13374	0	12325	55	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 2.

All (55) 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:D:736:ASN:HD21	1:D:854:MET:HE3	1.16	1.08
1:D:751:ALA:HB2	1:D:854:MET:CE	1.87	1.04
1:D:736:ASN:ND2	1:D:854:MET:HE3	1.73	1.03
1:D:751:ALA:HB2	1:D:854:MET:HE2	1.48	0.93
1:D:736:ASN:HD21	1:D:854:MET:CE	1.92	0.81
1:D:751:ALA:HB2	1:D:854:MET:HE1	1.62	0.80
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:ND2	2.25	0.69
1:C:771[A]:ASN:CG	1:D:771[A]:ASN:HD21	1.98	0.67
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:OD1	2.30	0.64
1:C:771[A]:ASN:HD21	1:D:771[A]:ASN:CG	2.02	0.62
1:B:595:ARG:HD2	1:B:681:LEU:HD22	1.82	0.60
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:HD21	2.04	0.55
1:A:606:LYS:HD2	1:A:638:ILE:HD12	1.88	0.54
1:C:771[A]:ASN:HD21	1:D:771[A]:ASN:ND2	2.06	0.54
3:D:876:RIE:H7	3:D:876:RIE:H12B	1.89	0.54
1:B:606:LYS:HD2	1:B:638:ILE:HD12	1.90	0.53
3:C:876:RIE:H12B	3:C:876:RIE:H7	1.91	0.53
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:ND2	2.57	0.53
3:B:876:RIE:H7	3:B:876:RIE:H12B	1.90	0.53
3:A:876:RIE:H7	3:A:876:RIE:H12B	1.91	0.52
1:A:581:SER:OG	1:A:840:ARG:HD2	2.11	0.51
1:D:751:ALA:CB	1:D:854:MET:HE2	2.31	0.51
1:A:476:ILE:HG23	1:A:484:LEU:HD13	1.94	0.50
1:A:749:TYR:OH	1:C:749:TYR:OH	2.30	0.50
1:A:592:PRO:HD2	1:A:645:ILE:O	2.13	0.49
1:A:771:ASN:CG	1:B:771[B]:ASN:HD21	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:PRO:HD2	1:B:645:ILE:O	2.16	0.46
1:A:771:ASN:OD1	1:B:771[B]:ASN:ND2	2.43	0.46
1:D:592:PRO:HD2	1:D:645:ILE:O	2.16	0.45
1:A:482:GLU:HB3	1:A:488:HIS:HD2	1.82	0.44
1:C:499:LEU:HD22	1:C:531:ILE:HG21	2.00	0.44
1:A:638:ILE:HG13	1:A:643:LEU:HD13	2.00	0.43
1:B:560:GLY:O	1:B:561:CYS:HB2	2.18	0.42
3:B:876:RIE:H16B	3:B:876:RIE:H14	1.79	0.42
1:C:592:PRO:HD2	1:C:645:ILE:O	2.19	0.42
1:C:774:SER:HA	1:C:799:SER:O	2.19	0.42
1:D:606:LYS:HD2	1:D:638:ILE:HD12	2.00	0.42
1:A:485:ILE:HG21	1:A:490:ARG:HD3	2.00	0.42
1:B:596:LEU:HD13	1:B:602:SER:HA	2.01	0.42
1:D:499:LEU:HD22	1:D:531:ILE:HG21	2.01	0.42
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:CG	2.71	0.42
1:D:736:ASN:ND2	1:D:854:MET:CE	2.60	0.42
1:A:793:ILE:HD13	1:A:851:LEU:HG	2.02	0.42
1:B:774:SER:HA	1:B:799:SER:O	2.20	0.41
1:A:451:ILE:HG23	1:A:457:LYS:HD3	2.02	0.41
1:A:560:GLY:O	1:A:561:CYS:HB2	2.19	0.41
1:A:477:PRO:HG2	1:A:480:LYS:HB2	2.03	0.41
1:C:637:SER:HB2	1:C:687:TYR:OH	2.20	0.41
3:A:876:RIE:H14	3:A:876:RIE:H16B	1.80	0.41
1:B:738:VAL:O	1:B:742:MET:HG2	2.21	0.41
3:A:876:RIE:H21	1:B:853:LEU:HD11	2.02	0.41
1:A:635:HIS:HB3	1:A:646:ARG:HB3	2.03	0.40
1:D:462:LEU:HD22	1:D:466:GLU:HG2	2.02	0.40
3:C:876:RIE:H16B	3:C:876:RIE:H14	1.79	0.40
1:D:560:GLY:O	1:D:561:CYS:HB2	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	Percentiles	
1	A	418/441 (95%)	405 (97%)	13 (3%)	0	100	100
1	B	401/441 (91%)	388 (97%)	13 (3%)	0	100	100
1	C	401/441 (91%)	387 (96%)	14 (4%)	0	100	100
1	D	393/441 (89%)	381 (97%)	12 (3%)	0	100	100
All	All	1613/1764 (91%)	1561 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	334/355 (94%)	331 (99%)	3 (1%)	84	76
1	B	325/355 (92%)	322 (99%)	3 (1%)	84	76
1	C	324/355 (91%)	320 (99%)	4 (1%)	78	65
1	D	315/355 (89%)	312 (99%)	3 (1%)	82	72
All	All	1298/1420 (91%)	1285 (99%)	13 (1%)	82	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	MET
1	A	657	MET
1	A	752	HIS
1	B	630	ARG
1	B	657	MET
1	B	752	HIS
1	C	464	ASP
1	C	486	GLU
1	C	657	MET
1	C	752	HIS
1	D	630	ARG
1	D	657	MET
1	D	752	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	B	488	HIS
1	B	510	GLN
1	B	658	ASN
1	C	635	HIS
1	D	510	GLN
1	D	635	HIS
1	D	736	ASN

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)

8 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	1	-	4,4,4	0.22	0	6,6,6	0.07	0
3	RIE	A	876	-	34,40,40	1.87	4 (11%)	40,56,56	1.85	8 (20%)
2	SO4	B	2	-	4,4,4	0.23	0	6,6,6	0.07	0
3	RIE	B	876	-	34,40,40	1.87	4 (11%)	40,56,56	1.84	9 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	3	-	4,4,4	0.24	0	6,6,6	0.09	0
3	RIE	C	876	-	34,40,40	1.86	4 (11%)	40,56,56	1.83	9 (22%)
2	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.11	0
3	RIE	D	876	-	34,40,40	1.87	4 (11%)	40,56,56	1.83	8 (20%)

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	1	-	-	0/0/0/0	0/0/0/0
3	RIE	A	876	-	-	0/31/37/37	0/3/3/3
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
3	RIE	B	876	-	-	0/31/37/37	0/3/3/3
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
3	RIE	C	876	-	-	0/31/37/37	0/3/3/3
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
3	RIE	D	876	-	-	0/31/37/37	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	876	RIE	C27-N3	-4.82	1.34	1.44
3	B	876	RIE	C27-N3	-4.69	1.34	1.44
3	D	876	RIE	C27-N3	-4.68	1.34	1.44
3	C	876	RIE	C27-N3	-4.66	1.34	1.44
3	D	876	RIE	C5-C6	-2.71	1.49	1.53
3	B	876	RIE	C5-C6	-2.69	1.49	1.53
3	A	876	RIE	C5-C6	-2.69	1.49	1.53
3	C	876	RIE	C5-C6	-2.60	1.49	1.53
3	A	876	RIE	C2-C5	4.21	1.50	1.40
3	C	876	RIE	C2-C5	4.22	1.50	1.40
3	B	876	RIE	C2-C5	4.29	1.50	1.40
3	D	876	RIE	C2-C5	4.32	1.50	1.40
3	A	876	RIE	C4-C5	7.47	1.50	1.38
3	B	876	RIE	C4-C5	7.52	1.50	1.38
3	C	876	RIE	C4-C5	7.55	1.50	1.38
3	D	876	RIE	C4-C5	7.55	1.50	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	876	RIE	C5-C4-N3	-4.97	103.43	106.67
3	D	876	RIE	C5-C4-N3	-4.91	103.47	106.67
3	B	876	RIE	C5-C4-N3	-4.70	103.61	106.67
3	C	876	RIE	C5-C4-N3	-4.57	103.69	106.67
3	D	876	RIE	C18-C27-C21	-3.64	115.56	121.21
3	B	876	RIE	C18-C27-C21	-3.58	115.65	121.21
3	C	876	RIE	C18-C27-C21	-3.58	115.65	121.21
3	A	876	RIE	C18-C27-C21	-3.49	115.79	121.21
3	D	876	RIE	C24-C30-C15	-2.46	119.33	122.87
3	B	876	RIE	C24-C30-C15	-2.44	119.36	122.87
3	C	876	RIE	C24-C30-C15	-2.42	119.39	122.87
3	A	876	RIE	C24-C30-C15	-2.31	119.54	122.87
3	C	876	RIE	C10-C11-C35	-2.24	108.67	112.94
3	B	876	RIE	C10-C11-C35	-2.23	108.68	112.94
3	A	876	RIE	C10-C11-C35	-2.19	108.76	112.94
3	D	876	RIE	C10-C11-C35	-2.14	108.85	112.94
3	B	876	RIE	C18-C27-N3	2.12	122.41	119.50
3	C	876	RIE	C18-C27-N3	2.12	122.41	119.50
3	A	876	RIE	C15-C18-C27	3.29	122.58	119.23
3	B	876	RIE	C15-C18-C27	3.34	122.63	119.23
3	D	876	RIE	C15-C18-C27	3.44	122.73	119.23
3	C	876	RIE	C15-C18-C27	3.45	122.74	119.23
3	C	876	RIE	C7-C4-N3	3.55	126.94	121.95
3	A	876	RIE	C24-C21-C27	3.58	122.88	119.23
3	C	876	RIE	C24-C21-C27	3.64	122.94	119.23
3	D	876	RIE	C7-C4-N3	3.65	127.08	121.95
3	B	876	RIE	C7-C4-N3	3.66	127.09	121.95
3	B	876	RIE	C24-C21-C27	3.68	122.98	119.23
3	D	876	RIE	C24-C21-C27	3.72	123.02	119.23
3	A	876	RIE	C7-C4-N3	3.86	127.38	121.95
3	D	876	RIE	C32-C1-N2	4.29	115.78	109.58
3	B	876	RIE	C32-C1-N2	4.50	116.10	109.58
3	A	876	RIE	C32-C1-N2	4.64	116.29	109.58
3	C	876	RIE	C32-C1-N2	4.64	116.30	109.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	876	RIE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	876	RIE	2	0
3	C	876	RIE	2	0
3	D	876	RIE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	420/441 (95%)	0.60	40 (9%) 10 11	14, 23, 49, 69	0
1	B	405/441 (91%)	0.77	45 (11%) 7 8	14, 23, 81, 109	0
1	C	404/441 (91%)	0.67	45 (11%) 7 8	13, 22, 80, 101	0
1	D	394/441 (89%)	0.60	36 (9%) 11 13	13, 22, 45, 94	0
All	All	1623/1764 (92%)	0.66	166 (10%) 9 9	13, 23, 61, 109	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	LEU	16.4
1	B	452	LEU	16.4
1	D	484	LEU	14.1
1	B	461	PHE	13.5
1	A	455	ALA	12.0
1	B	444	PRO	11.0
1	B	450	GLN	10.7
1	C	484	LEU	10.7
1	B	451	ILE	9.9
1	D	469	GLN	9.8
1	D	470	LEU	9.6
1	B	473	ALA	9.6
1	C	461	PHE	9.2
1	D	472	ASN	9.0
1	A	453	GLY	8.9
1	C	483	THR	8.8
1	B	474	LYS	8.6
1	C	471	VAL	8.6
1	B	447	GLU	8.0
1	D	468	ILE	7.8
1	B	448	CYS	7.6

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Mol	Chain	Res	Type	RSRZ
1	D	471	VAL	7.6
1	D	458	GLY	7.5
1	A	461	PHE	7.5
1	D	461	PHE	7.4
1	D	486	GLU	7.3
1	C	444	PRO	7.1
1	D	483	THR	6.9
1	B	484	LEU	6.8
1	B	445	ASN	6.8
1	A	441	GLU	6.7
1	C	470	LEU	6.6
1	D	485	ILE	6.6
1	C	458	GLY	6.5
1	A	442	PRO	6.4
1	B	471	VAL	6.3
1	C	462	LEU	6.2
1	B	446	GLU	6.0
1	A	454	ASN	5.9
1	C	451	ILE	5.5
1	C	482	GLU	5.4
1	C	452	LEU	5.3
1	D	462	LEU	5.3
1	C	450	GLN	5.2
1	C	445	ASN	5.1
1	A	446	GLU	5.1
1	C	486	GLU	5.1
1	D	487	THR	5.0
1	D	459	ALA	4.9
1	A	633	LYS	4.6
1	B	470	LEU	4.5
1	C	453	GLY	4.5
1	A	450	GLN	4.5
1	A	523	MET	4.5
1	C	468	ILE	4.4
1	B	462	LEU	4.4
1	B	485	ILE	4.4
1	D	466	GLU	4.4
1	B	442	PRO	4.2
1	C	448	CYS	4.2
1	D	786	PRO	4.2
1	C	487	THR	4.2
1	C	829	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	449	LEU	4.0
1	B	468	ILE	4.0
1	C	469	GLN	4.0
1	B	486	GLU	4.0
1	D	465	ALA	4.0
1	B	523	MET	3.9
1	C	467	ILE	3.8
1	B	472	ASN	3.8
1	A	462	LEU	3.8
1	A	456	GLU	3.7
1	A	457	LYS	3.7
1	A	449	LEU	3.7
1	D	630	ARG	3.7
1	A	650	ARG	3.7
1	C	460	LYS	3.6
1	B	460	LYS	3.6
1	A	452	LEU	3.6
1	B	459	ALA	3.6
1	B	633	LYS	3.6
1	A	630	ARG	3.5
1	C	446	GLU	3.5
1	A	444	PRO	3.5
1	C	447	GLU	3.4
1	A	485	ILE	3.4
1	B	467	ILE	3.4
1	B	469	GLN	3.4
1	D	467	ILE	3.4
1	C	463	SER	3.4
1	C	630	ARG	3.4
1	B	829	ASP	3.3
1	A	828	LYS	3.3
1	D	829	ASP	3.3
1	D	633	LYS	3.2
1	D	463	SER	3.2
1	C	860	GLY	3.1
1	A	483	THR	3.1
1	D	464	ASP	3.0
1	C	459	ALA	3.0
1	C	485	ILE	2.9
1	B	464	ASP	2.9
1	B	787	THR	2.9
1	D	828	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	443	ARG	2.8
1	B	466	GLU	2.8
1	A	501	LYS	2.7
1	C	633	LYS	2.7
1	B	650	ARG	2.7
1	A	658	ASN	2.7
1	B	441	GLU	2.7
1	A	786	PRO	2.7
1	C	628	PHE	2.7
1	B	828	LYS	2.7
1	A	468	ILE	2.6
1	C	454	ASN	2.6
1	B	524	GLY	2.6
1	C	786	PRO	2.6
1	D	571	ARG	2.5
1	D	516	ASP	2.5
1	B	501	LYS	2.5
1	D	523	MET	2.5
1	A	600	CYS	2.5
1	A	498	LEU	2.5
1	D	627	ARG	2.4
1	C	828	LYS	2.4
1	A	460	LYS	2.4
1	C	490	ARG	2.3
1	A	787	THR	2.3
1	A	486	GLU	2.3
1	C	657	MET	2.2
1	D	659	MET	2.2
1	D	620	GLU	2.2
1	A	515	ARG	2.2
1	D	658	ASN	2.2
1	B	718	ARG	2.2
1	B	666	LYS	2.2
1	D	830	ASN	2.2
1	D	490	ARG	2.2
1	A	475	HIS	2.2
1	B	600	CYS	2.2
1	A	447	GLU	2.2
1	A	524	GLY	2.2
1	A	860	GLY	2.2
1	A	484	LEU	2.1
1	C	681	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	630	ARG	2.1
1	B	860	GLY	2.1
1	B	465	ALA	2.1
1	D	460	LYS	2.1
1	C	505	GLU	2.1
1	B	488	HIS	2.1
1	C	718	ARG	2.1
1	C	465	ALA	2.1
1	D	482	GLU	2.1
1	D	613	GLU	2.1
1	A	666	LYS	2.1
1	A	789	GLU	2.1
1	C	785	GLY	2.1
1	C	515	ARG	2.1
1	B	463	SER	2.0
1	A	829	ASP	2.0
1	A	708	CYS	2.0
1	C	598	ARG	2.0
1	C	787	THR	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, 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	B	2	5/5	0.85	0.21	2.96	58,58,58,58	0
3	RIE	A	876	38/38	0.90	0.12	1.91	16,21,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	1	5/5	0.83	0.20	1.44	47,47,47,47	0
3	RIE	B	876	38/38	0.93	0.10	0.69	16,22,23,24	0
3	RIE	C	876	38/38	0.92	0.11	0.63	15,20,22,22	0
3	RIE	D	876	38/38	0.93	0.10	0.57	16,20,22,22	0
2	SO4	C	3	5/5	0.93	0.13	0.09	42,42,42,42	0
2	SO4	D	4	5/5	0.95	0.12	-0.20	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.